

## EAST Search History

Ref #	Hits	Search Query	DBs	Default Operator	Plurals	Time Stamp
L1	551500	phenyl	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	ON	2007/12/11 07:53
L2	2479	hexenoic	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	ON	2007/12/11 07:53
L3	40	L2 near5 L1	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	ON	2007/12/11 07:53
L4	176	(562/491).CCLS.	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	OFF	2007/12/11 07:53
L5	1461	(514/562).CCLS.	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	OFF	2007/12/11 07:53
L6	601	(514/564).CCLS.	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	OFF	2007/12/11 07:53
L7	1167	(514/570).CCLS.	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	OFF	2007/12/11 07:53
L8	361	(514/571).CCLS.	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	OFF	2007/12/11 07:53
L9	241	(562/495).CCLS.	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	OFF	2007/12/11 07:53
L10	654	(514/559).CCLS.	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	OFF	2007/12/11 07:53
L11	4257	L4 or L9 or L10 or L5 or L6 or L7 or L8	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	ON	2007/12/11 07:53

## EAST Search History

L12	1	L3 and L11	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	ON	2007/12/11 07:53
L13	164286	cyclohexyl	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	ON	2007/12/11 07:53
L14	17	L3 and L13	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	ON	2007/12/11 07:53
L15	11	("4513005").URPN.	USPAT	OR	ON	2007/12/11 07:53
L16	0	"49047735"	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	ON	2007/12/11 07:54
L17	0	("49047735").PN.	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	OFF	2007/12/11 07:55
L18	82	heptatrienoic	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	ON	2007/12/11 07:56
L19	23	I1 near20 I18	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	ON	2007/12/11 08:02
L20	666	pentadienoic	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	ON	2007/12/11 08:10
L21	93	I1 near20 I20	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	ON	2007/12/11 08:06
L22	35	"112429"	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	ON	2007/12/11 08:06
L23	197168	("514").CLAS.	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	OFF	2007/12/11 08:10
L24	164	I20 and I23	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	ON	2007/12/11 08:29

## EAST Search History

L25	2	("5675033").PN.	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	OFF	2007/12/11 08:13
L26	14	"6238649"	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	ON	2007/12/11 10:11
L27	2	("5010189").PN.	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	OFF	2007/12/11 10:11

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TERMINAL (ENTER 1, 2, 3, OR ?):2

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NEWS	1		Web Page for STN Seminar Schedule - N. America
NEWS	2	JUL 02	LMEDLINE coverage updated
NEWS	3	JUL 02	SCISEARCH enhanced with complete author names
NEWS	4	JUL 02	CHEMCATS accession numbers revised
NEWS	5	JUL 02	CA/CAPplus enhanced with utility model patents from China
NEWS	6	JUL 16	CAplus enhanced with French and German abstracts
NEWS	7	JUL 18	CA/CAPplus patent coverage enhanced
NEWS	8	JUL 26	USPATFULL/USPAT2 enhanced with IPC reclassification
NEWS	9	JUL 30	USGENE now available on STN
NEWS	10	AUG 06	CAS REGISTRY enhanced with new experimental property tags
NEWS	11	AUG 06	FSTA enhanced with new thesaurus edition
NEWS	12	AUG 13	CA/CAPplus enhanced with additional kind codes for granted patents
NEWS	13	AUG 20	CA/CAPplus enhanced with CAS indexing in pre-1907 records
NEWS	14	AUG 27	Full-text patent databases enhanced with predefined patent family display formats from INPADOCDB
NEWS	15	AUG 27	USPATOLD now available on STN
NEWS	16	AUG 28	CAS REGISTRY enhanced with additional experimental spectral property data
NEWS	17	SEP 07	STN AnaVist, Version 2.0, now available with Derwent World Patents Index
NEWS	18	SEP 13	FORIS renamed to SOFIS
NEWS	19	SEP 13	INPADOCDB enhanced with monthly SDI frequency
NEWS	20	SEP 17	CA/CAPplus enhanced with printed CA page images from 1967-1998
NEWS	21	SEP 17	CAplus coverage extended to include traditional medicine patents
NEWS	22	SEP 24	EMBASE, EMBAL, and LEMBASE reloaded with enhancements
NEWS	23	OCT 02	CA/CAPplus enhanced with pre-1907 records from Chemisches Zentralblatt
NEWS	24	OCT 19	BEILSTEIN updated with new compounds
NEWS	25	NOV 15	Derwent Indian patent publication number format enhanced
NEWS	26	NOV 19	WPIX enhanced with XML display format
NEWS	27	NOV 30	ICSD reloaded with enhancements
NEWS	28	DEC 04	LINPADOCDB now available on STN
NEWS EXPRESS	19	SEPTEMBER 2007: CURRENT WINDOWS VERSION IS V8.2, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 19 SEPTEMBER 2007.	
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NEWS LOGIN	Welcome Banner and News Items		
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FILE 'HOME' ENTERED AT 06:07:53 ON 11 DEC 2007

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

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<http://www.cas.org/support/stngen/stndoc/properties.html>

=> 2,4-pentadieneoic acid/cn

L1 0 2,4-PENTADIENEOIC ACID/CN

=> e 2,4-pentadieneoic acid/cn

E1	1	2,4-PENTADIENENITRILE-5-D, 5-(6,6-DIMETHYL-1-CYCLOHEXEN-1-YL-2-D)-3-METHYL-, (E,E)-/CN
E2	1	2,4-PENTADIENENITRILE-5-D, 5-(6,6-DIMETHYL-1-CYCLOHEXEN-1-YL-2-D)-3-METHYL-, (Z,E)-/CN
E3	0 -->	2,4-PENTADIENEOIC ACID/CN
E4	1	2,4-PENTADIENEPEEROXOIC ACID, 5-PHENYL-, 1,1-DIMETHYLETHYL ESTER/CN
E5	1	2,4-PENTADIENESELENOAMIDE, 2-(1,1-DIMETHYLETHYL)-N,N-DIETHYL-/CN
E6	1	2,4-PENTADIENESELENOAMIDE, N,N-DIETHYL-2-(TRIMETHYLSILYL)-/CN
E7	1	2,4-PENTADIENESELENOAMIDE, N,N-DIETHYL-3-METHYL-2-(TRIMETHYLSILYL)-, (E)-/CN
E8	1	2,4-PENTADIENESELENOAMIDE, N,N-DIETHYL-3-METHYL-2-(TRIMETHYLSILYL)-, (Z)-/CN
E9	1	2,4-PENTADIENETHIAL/CN
E10	1	2,4-PENTADIENETHIAL, (Z)-/CN
E11	1	2,4-PENTADIENETHIAL, 2-METHYL-/CN
E12	1	2,4-PENTADIENETHIAL, 3-HYDROXY-/CN

=> e 2,4-pentadienoic acid/cn

E1	1	2,4-PENTADIENOIC ACID, 4-METHYL-5-(5-NITRO-2-FURYL)-/CN
E2	1	2,4-PENTADIENOIC ACID, N,5-DIPHENYL-/CN
E3	1 -->	2,4-PENTADIENOIC ACID/CN
E4	1	2,4-PENTADIENOIC ACID AMIDE/CN
E5	1	2,4-PENTADIENOIC ACID N-METHYLAMIDE/CN
E6	1	2,4-PENTADIENOIC ACID, (1R,2S)-2-PHENYLCYCLOHEXYL ESTER, (2E)-REL-/CN
E7	1	2,4-PENTADIENOIC ACID, (1R,2S,5R)-5-METHYL-2-(1-METHYL-1-PHENYLETHYL)CYCLOHEXYL ESTER, (2E)-REL-/CN
E8	1	2,4-PENTADIENOIC ACID, (1R,2S,5R)-5-METHYL-2-(1-METHYLETHYL)CYCLOHEXYL ESTER, (2E)-/CN
E9	1	2,4-PENTADIENOIC ACID, (2E)-/CN
E10	1	2,4-PENTADIENOIC ACID, (2E)-, COMPD. WITH 1-NAPHTHALENEMETHANAMINE (1:1)/CN
E11	1	2,4-PENTADIENOIC ACID, (2E)-, COMPD. WITH 1-NAPHTHALENEMETHANAMINE (1:1), HOMOPOLYMER/CN
E12	1	2,4-PENTADIENOIC ACID, (2E)-2,4-PENTADIENYL ESTER, (2E)-/CN

=> e 2,4-pentadienoic acid, 5-methyl/cn

E1	1	2,4-PENTADIENOIC ACID, 5-METHOXY-3-(PHENYLTHIO)-5-((TRIMETHYLSILYL)OXY)-, METHYL ESTER/CN
E2	1	2,4-PENTADIENOIC ACID, 5-METHOXY-3-METHYL-, METHYL ESTER/CN
E3	0 -->	2,4-PENTADIENOIC ACID, 5-METHYL/CN
E4	1	2,4-PENTADIENOIC ACID, 5-METHYL-2-(1-METHYL-1-PHENYLETHYL)CYCLOHEXYL ESTER, (1R-(1A,2B,5A))-/CN
E5	1	2,4-PENTADIENOIC ACID, 5-METHYL-2-(1-METHYLETHYL)CYCLOHEXYL ESTER, (1R-(1A,2B,5A))-/CN
E6	1	2,4-PENTADIENOIC ACID, 5-NITRO-/CN
E7	1	2,4-PENTADIENOIC ACID, 5-NITRO-, (2E,4E)-/CN
E8	1	2,4-PENTADIENOIC ACID, 5-NITRO-, ETHYL ESTER/CN
E9	1	2,4-PENTADIENOIC ACID, 5-NITRO-, ETHYL ESTER, (E,E)-/CN
E10	1	2,4-PENTADIENOIC ACID, 5-NITRO-, ION(1-)/CN
E11	1	2,4-PENTADIENOIC ACID, 5-NITRO-, METHYL ESTER, (E,E)-/CN
E12	1	2,4-PENTADIENOIC ACID, 5-OXIRANYL-, METHYL ESTER, (E,E)-/CN

=> logoff hold

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	7.20	7.41

SESSION WILL BE HELD FOR 120 MINUTES  
STN INTERNATIONAL SESSION SUSPENDED AT 06:10:59 ON 11 DEC 2007

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PASSWORD:

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SESSION RESUMED IN FILE 'REGISTRY' AT 06:15:06 ON 11 DEC 2007  
FILE 'REGISTRY' ENTERED AT 06:15:06 ON 11 DEC 2007  
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COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
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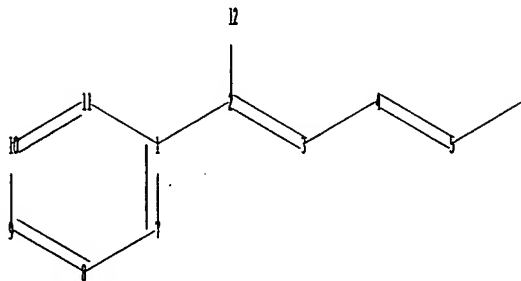
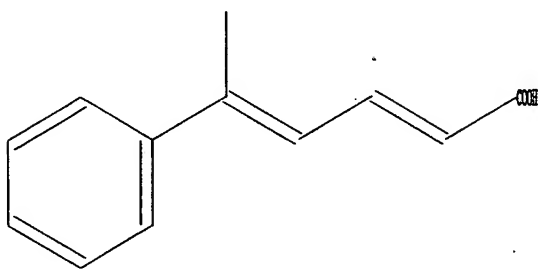
FULL ESTIMATED COST

7.20

7.41

=>

Uploading C:\Documents and Settings\PZucker\My Documents\Examination Auxillary files\10025947\10025947 pt V stab 1.str



chain nodes :

2 3 4 5 6 12

ring nodes :

1 7 8 9 10 11

chain bonds :

1-2 2-3 2-12 3-4 4-5 5-6

ring bonds :

1-7 1-11 7-8 8-9 9-10 10-11

exact bonds :

1-2 2-3 2-12 3-4 4-5 5-6

normalized bonds :

1-7 1-11 7-8 8-9 9-10 10-11

Match level :

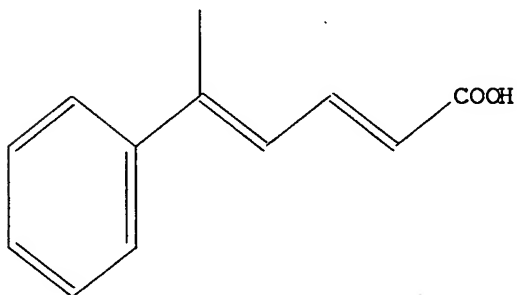
1:Atom 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:Atom 8:Atom 9:Atom  
10:Atom 11:Atom 12:CLASS

L2 STRUCTURE UPLOADED

=> d 12

L2 HAS NO ANSWERS

L2 STR



Structure attributes must be viewed using STN Express query preparation.

=> search 12 exact sam

SAMPLE SEARCH INITIATED 06:16:19 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 9 TO ITERATE

100.0% PROCESSED

9 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 9 TO 360  
PROJECTED ANSWERS: 0 TO 0

L3 0 SEA EXA SAM L2

=> search l2 exact full

FULL SEARCH INITIATED 06:16:26 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 115 TO ITERATE

100.0% PROCESSED 115 ITERATIONS  
SEARCH TIME: 00.00.01

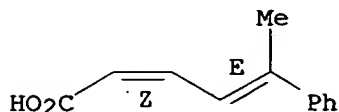
3 ANSWERS

L4 3 SEA EXA FUL L2

=> d scan

L4 3 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN  
IN 2,4-Hexadienoic acid, 5-phenyl-, (Z,E)- (9CI)  
MF C12 H12 O2

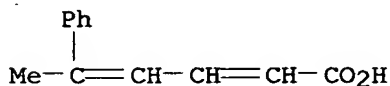
Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):3

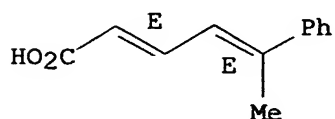
L4 3 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN  
IN Sorbic acid, 5-phenyl- (6CI)  
MF C12 H12 O2



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 3 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN  
IN 2,4-Hexadienoic acid, 5-phenyl-, (E,E)- (9CI)  
MF C12 H12 O2

Double bond geometry as shown.





\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

ALL ANSWERS HAVE BEEN SCANNED

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

66.35

66.56

FILE 'CAPLUS' ENTERED AT 06:16:55 ON 11 DEC 2007

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=> 14

L5 9 L4

=> d 15 1-9 ti

L5 ANSWER 1 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN

TI Structure-antitranspirant activity relation in a series of abscisic acid analogs

L5 ANSWER 2 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN

TI Influence of the substituent and the geometry of the double bond on dissociation constants of cinnamylideneacetic acids

L5 ANSWER 3 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN

TI Several dichlorobutadienyl alcohols and their transformation into dienic acids

L5 ANSWER 4 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN

TI Synthesis of polyene acids and aldehydes derived from dichloroacrolein

L5 ANSWER 5 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN

TI Ketones with a cyclopropane nucleus. II. Some 2-oxobenzobicyclo[0.1.4]hept-3-ene compounds substituted in position 5

L5 ANSWER 6 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN

TI Ketones with a cyclopropane nucleus. I. Benzo- and

naphthobicyclo[0.1.4]heptenones

L5 ANSWER 7 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN  
TI Hydroxytriazenes of anthraquinone

L5 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN  
TI Stereochemistry of the 1-methyl-2-carboxy-1,2,3,4-tetrahydronaphthalenes  
and the 5-methylbenzobicyclo[0.1.4]-hept-3-en-2-ones

L5 ANSWER 9 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN  
TI Reformatskii reactions with methyl  $\gamma$ -bromocrotonate

=> file reg  
COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
11.52	78.08

FULL ESTIMATED COST

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=> file caplus  
COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
0.45	78.53

FULL ESTIMATED COST

FILE 'CAPLUS' ENTERED AT 06:28:11 ON 11 DEC 2007  
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FILE LAST UPDATED: 10 Dec 2007 (20071210/ED)

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=> d his

(FILE 'HOME' ENTERED AT 06:07:53 ON 11 DEC 2007)

FILE 'REGISTRY' ENTERED AT 06:08:12 ON 11 DEC 2007

L1 0 2,4-PENTADIENEOIC ACID/CN  
E 2,4-PENTADIENEOIC ACID/CN  
E 2,4-PENTADIENEOIC ACID/CN  
E 2,4-PENTADIENEOIC ACID, 5-METHYL/CN  
L2 STRUCTURE UPLOADED  
L3 0 SEARCH L2 EXACT SAM  
L4 3 SEARCH L2 EXACT FULL

FILE 'CAPLUS' ENTERED AT 06:16:55 ON 11 DEC 2007

L5 9 L4

FILE 'REGISTRY' ENTERED AT 06:27:46 ON 11 DEC 2007

FILE 'CAPLUS' ENTERED AT 06:28:11 ON 11 DEC 2007

=> file reg

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FULL ESTIMATED COST	0.47	79.00

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experimental property data in the original document. For information  
on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=> e 2,4-pentadienoic acid/cn

E1 1 2,4-PENTADIENOHYDROXAMIC ACID, 4-METHYL-5-(5-NITRO-2-FURYL)-  
/CN  
E2 1 2,4-PENTADIENOHYDROXAMIC ACID, N,5-DIPHENYL-/CN

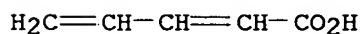
E3 1 --> 2,4-PENTADIENOIC ACID/CN  
 E4 1 2,4-PENTADIENOIC ACID AMIDE/CN  
 E5 1 2,4-PENTADIENOIC ACID N-METHYLAMIDE/CN  
 E6 1 2,4-PENTADIENOIC ACID, (1R,2S)-2-PHENYLCYCLOHEXYL ESTER, (2E)  
 )-REL-/CN  
 E7 1 2,4-PENTADIENOIC ACID, (1R,2S,5R)-5-METHYL-2-(1-METHYL-1-PHE  
 NYLETHYL)CYCLOHEXYL ESTER, (2E)-REL-/CN  
 E8 1 2,4-PENTADIENOIC ACID, (1R,2S,5R)-5-METHYL-2-(1-METHYLETHYL)  
 CYCLOHEXYL ESTER, (2E)-/CN  
 E9 1 2,4-PENTADIENOIC ACID, (2E)-/CN  
 E10 1 2,4-PENTADIENOIC ACID, (2E)-, COMPD. WITH 1-NAPHTHALENEMETHA  
 NAMINE (1:1)/CN  
 E11 1 2,4-PENTADIENOIC ACID, (2E)-, COMPD. WITH 1-NAPHTHALENEMETHA  
 NAMINE (1:1), HOMOPOLYMER/CN  
 E12 1 2,4-PENTADIENOIC ACID, (2E)-2,4-PENTADIENYL ESTER, (2E)-/CN

=> e3

L6 1 "2,4-PENTADIENOIC ACID"/CN

=> d 16

L6 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2007 ACS on STN  
 RN 626-99-3 REGISTRY  
 ED Entered STN: 16 Nov 1984  
 CN 2,4-Pentadienoic acid (CA INDEX NAME)  
 OTHER CA INDEX NAMES:  
 CN  $\alpha,\gamma$ -Pentadienoic acid (3CI)  
 OTHER NAMES:  
 CN  $\beta$ -Vinylacrylic acid  
 CN 1,3-Butadiene-1-carboxylic acid  
 CN 1-Carboxy-1,3-butadiene  
 CN 1-Carboxybutadiene  
 CN Butadiene-1-carboxylic acid  
 CN NSC 16628  
 MF C5 H6 O2  
 CI COM  
 LC STN Files: BEILSTEIN\*, BIOSIS, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS,  
 CHEMINFORMRX, CHEMLIST, CSCHEM, DETHERM\*, IFICDB, IFIPAT, IFIUDB,  
 SPECINFO, TOXCENTER, USPAT2, USPATFULL, USPATOLD  
 (\*File contains numerically searchable property data)  
 Other Sources: EINECS\*\*  
 (\*\*Enter CHEMLIST File for up-to-date regulatory information)



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

155 REFERENCES IN FILE CA (1907 TO DATE)  
 14 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA  
 156 REFERENCES IN FILE CAPLUS (1907 TO DATE)  
 12 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	7.35	86.35

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FILE COVERS 1907 - 11 Dec 2007 VOL 147 ISS 25  
FILE LAST UPDATED: 10 Dec 2007 (20071210/ED)

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=> 16/thu

156 L6  
960327 THU/RL  
L7 2 L6/THU  
(L6 (L) THU/RL)

=> d 17 1-2 ti fbib abs

L7 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2007 ACS on STN  
TI Use of pentadienoic acid derivatives for the treatment of hyperuricemia  
AN 2005:523273 CAPLUS  
DN 143:53517  
TI Use of pentadienoic acid derivatives for the treatment of hyperuricemia  
IN Boizel, Robert; Fouqueray, Pascale; Guerrier, Daniel; Zeiller, Jean-Jacques; Brutzkus, Bertrand  
PA Merck Patent G.m.b.H., Germany  
SO PCT Int. Appl., 64 pp.  
CODEN: PIXXD2  
DT Patent  
LA English  
FAN.CNT 2

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IN 2006KN00961	A	20070420	IN 2006-KN961	20060418
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			WO 2004-EP12381	W 20041102

PATENT FAMILY INFORMATION:

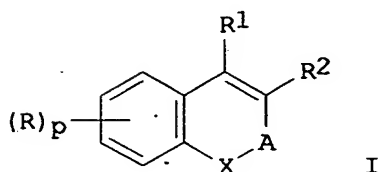
FAN 2005:467780

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			US 2003-527773P	P	20031209
			WO 2004-EP12381	W	20041102

OS MARPAT 143:53517  
 GI



AB The use of a pentadienoic acid derivative of formula I (e.g., (2E,4E)-5-(3,3-dimethyl-7-methoxy-2,3-dihydrobenzoxepin-5-yl)-3-methylpenta-2,4-dienoic acid) is claimed for the preparation of a medicament for the prevention or treatment of hyperuricemia and/or one or several associated disorders or diseases, and/or for reducing the serum uric acid level of a subject. Medical compns. for these prevention and/or treatment, comprising such a pentadienoic acid derivative

RE.CNT 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD

## ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2007 ACS on STN  
 TI Use of pentadienoic acid derivatives for the prevention and/or the  
 treatment of hyperuricemia  
 AN 2005:467780 CAPLUS  
 DN 143:1300  
 TI Use of pentadienoic acid derivatives for the prevention and/or the  
 treatment of hyperuricemia  
 IN Boizel, Robert; Fouqueray, Pascale; Guerrier, Daniel; Zeller,  
 Jean-Jacques; Brutzkus, Bertrand  
 PA Merck Sante, Fr.  
 SO Eur. Pat. Appl., 45 pp.  
 CODEN: EPXXDW  
 DT Patent  
 LA English  
 FAN.CNT 2

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PATENT FAMILY INFORMATION:

FAN 2005:523273

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			WO 2004-EP12381	W	20041102

OS MARPAT 143:1300

AB Use of pentadienoic acid derivs. for the prevention and/or the treatment of hyperuricemia and/or associated disorders or diseases. The use of a pentadienoic acid derivative of formula (I) for the preparation of a medicament for

the prevention or treatment of hyperuricemia and/or one or several associated disorders or diseases, and/or for reducing the serum uric acid level of a subject. Medical compns. for these prevention and/or treatment, comprising such a pentadienoic acid derivative

RE.CNT 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

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COST IN U.S. DOLLARS

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FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

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ENTRY	SESSION
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           (L6 (L) PREP/RL)

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L8 ANSWER 30 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN  
 TI Diene syntheses. XXVI. A dimeric butadiene-1-carboxylic acid

L8 ANSWER 31 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN  
 TI 2,4-Pentadienoic acids

L8 ANSWER 32 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN  
 TI Butadienyl compounds

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 TI A hypothesis on the biological origin of resin acids

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L8 ANSWER 28 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN  
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 AU Eglinton, G.; Jones, E. R. H.; Mansfield, G. H.; Whiting, M. C.

CS Univ. Manchester, UK  
 SO Journal of the Chemical Society (1954) 3197-3200  
 CODEN: JCSOA9; ISSN: 0368-1769  
 DT Journal  
 LA Unavailable  
 OS CASREACT 49:60249  
 AB cf. C.A. 49, 8142f. A study has been made of the effect of alkali on but-3-ynoic acid (I). Under the mild conditions of heating 3 hrs. at 40° with 18% K<sub>2</sub>CO<sub>3</sub> solution, a 92% yield of buta-2,3-dienoic acid (II), m. 65-6° (from light petroleum) was obtained. More vigorous treatment (18% K<sub>2</sub>CO<sub>3</sub> at 90° for 6 hrs.) gave further isomerization to but-2-ynoic acid (III), m. 75-6° (from light petroleum). Et but-3-ynoate (IV), b. 104-5°/190 mm., n<sub>D</sub> 1.4291, isomerized much more readily than the acid. Even KHCO<sub>3</sub> solution at 50° gave Et buta-2,3-dienoate (V), b. 44°/130 mm., n<sub>D</sub> 1.4585, and with 10% K<sub>2</sub>CO<sub>3</sub> at 20°, the reaction went almost to completion. V was found to be extremely reactive toward nucleophilic reagents. Treating V with an EtOH solution of NaOEt gave Et β-ethoxycrotonate (VI). Piperidine also added to V to form Et β-piperidinocrotonate, b. 110° (bath temperature)/0.03 mm., n<sub>D</sub> 1.5392, λ<sub>maximum</sub> 2870 Å., ε = 24700. V and aniline yielded Et β-anilinocrotonate, b. 106°/0.5 mm., n<sub>D</sub> 1.5820, λ<sub>maximum</sub> 3010 Å., ε = 20400, and with p-phenetidine and V, there resulted Et β-p-ethoxyanilinocrotonate, m. 53-4°, λ<sub>maximum</sub> 2960 Å., ε = 22800. When a solution of II in xylene was refluxed, there was gradual polymerization and a little dehydroacetic acid was isolated. Partial hydrogenation of II in EtOAc in the presence of 1.5% Pd on CaCO<sub>3</sub> gave cis-crotonic acid, which, on bromination, gave a 70% yield of threo-α,β-dibromobutyric acid, m. 58-9° (from pentane). Reaction of II and V with LiAlH<sub>4</sub> was also studied. II gave primarily vinylacetic acid, b. 85° (bath temperature)/16 mm., n<sub>D</sub> 1.4218, and some but-3-en-1-ol, b. 112°/767 mm., n<sub>D</sub> 1.4180; α-naphthylurethan, m. 76-7°. A similar reduction of V gave Et vinylacetate, b. 75°/130 mm., n<sub>D</sub> 1.4110, and a small quantity of but-3-en-1-ol.

L8 ANSWER 29 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN  
 TI 2,4-Pentadienoic acids  
 AN 1952:42374 CAPLUS  
 DN 46:42374  
 OREF 46:7114i  
 TI 2,4-Pentadienoic acids  
 PA N. V. de Bataafsche Petroleum Maatschappij  
 DT Patent  
 LA Unavailable  
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	GB 668569		19520319	GB 1949-18473	19490713
AB	See U.S. 2,515,595 (C.A. 44, 9979b).				

L8 ANSWER 30 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN  
 TI Diene syntheses. XXVI. A dimeric butadiene-1-carboxylic acid  
 AN 1951:26931 CAPLUS  
 DN 45:26931  
 OREF 45:4683e-i, 4684a-d  
 TI Diene syntheses. XXVI. A dimeric butadiene-1-carboxylic acid  
 AU Alder, Kurt; Vogt, Wilhelm  
 CS Univ. Cologne, Germany  
 SO Ann. (1950), 570, 190-200  
 DT Journal  
 LA Unavailable  
 GI For diagram(s), see printed CA Issue.  
 AB cf. C.A. 44, 1066a. Details are given for the preparation and purification of

CH<sub>2</sub>:CHCH:CHCO<sub>2</sub>H (I), b<sub>12</sub> 102-3°, m. 72°, formed from CH<sub>2</sub>(CO<sub>2</sub>H)<sub>2</sub> and acrolein. I (31 g.) refluxed 24 hrs. with 2% each methylene blue and p-(HO)2C<sub>6</sub>H<sub>4</sub> in 155 g. xylene, followed by extraction with hot aqueous Na<sub>2</sub>CO<sub>3</sub>, acidification, and extraction with Et<sub>2</sub>O gave about 40% of a crystalline dimer (II), m. 147° (from AcOEt), and 40% of an oily mixture (III), together with a tacky polymeric mixture II (2 g.) heated 2 hrs. with 3.3 g. Br at 200°, followed by solution in aqueous Na<sub>2</sub>CO<sub>3</sub>, filtration, and debromination with Na-Hg and treatment at 0° with 5% KMnO<sub>4</sub>, gave o-HO<sub>2</sub>CC<sub>6</sub>H<sub>4</sub>CH<sub>2</sub>CH<sub>2</sub>CO<sub>2</sub>H, m. 165-6° (cf. Straus and Lemmel, C.A. 7, 1499). II (0.5 g.) warmed 2-3 min. with 15 parts concentrated H<sub>2</sub>SO<sub>4</sub>, rapidly cooled, poured on ice, and extracted with Et<sub>2</sub>O gave a mixture of 1,2-C<sub>6</sub>H<sub>4</sub>.CO.O.CHCH<sub>2</sub>CO<sub>2</sub>H, m. 152° (cf. Roth, C.A. 8, 2724) and a new hydrindonecarboxylic acid, Cl<sub>10</sub>H<sub>8</sub>O<sub>3</sub> (IV), m. 222-3° (from AcOEt) (semicarbazone, decompose 285°), whose (impure) Me ester m. 102° [semicarbazone, Cl<sub>2</sub>H<sub>13</sub>O<sub>3</sub>N<sub>3</sub>, needles, decompose 259° (from AcOAm)]. Catalytic hydrogenation of II with PtO<sub>2</sub> in AcOH proceeded at a constant rate (indicating absence of appreciable amts. of an isomer) and yielded a cis-dihydro derivative (V) of II, m. 128°; Me ester, oil. Refluxed 8 hrs. with 5 cc. 40% KOH, 1 g. V gave, after acidification, trans-HO<sub>2</sub>CCCH<sub>2</sub>(CH<sub>2</sub>)<sub>4</sub>.CHCH:CHCO<sub>2</sub>H (VI), m. 180°, which oxidized with cold alkaline KMnO<sub>4</sub> gave 1,2-(HO<sub>2</sub>C)2C<sub>6</sub>H<sub>10</sub>, m. 219-20° (Diels and Alder, C.A. 22, 1144). Refluxing VI with 50 parts 10% H<sub>2</sub>SO<sub>4</sub> yielded the trans-lactone, Cl<sub>10</sub>H<sub>14</sub>O<sub>4</sub>, m. 119° and depressing the m.p. of V. Refluxing II 0.5 hr. with 5 parts 40% KOH, followed by acidification and Et<sub>2</sub>O extraction, gave the compound (VII), m. 136° and depressing the m.p. of II. When hydrogenated, VII gave V, but when II was refluxed 20 hrs. with 40% KOH, it yielded a dienedicarboxylic acid, HO<sub>2</sub>CC:C(CH:CHCO<sub>2</sub>H).CH<sub>2</sub>.CH<sub>2</sub>.CH<sub>2</sub>.CH<sub>2</sub> (VIII), m. (poorly due to lactonization) 158-63° (from AcOH), readily isomerized by hot aqueous H<sub>2</sub>SO<sub>4</sub> to CH<sub>2</sub>.(CH<sub>2</sub>)<sub>2</sub>.CH<sub>2</sub>.C:C.CH(CH<sub>2</sub>CO<sub>2</sub>H).O.CO, m. 114-15°. The latter was unsatd. toward KMnO<sub>4</sub>, but failed to add H at room temperature when treated with PtO<sub>2</sub> in AcOH. Under similar conditions, VIII proved difficult to hydrogenate; even after 3 days a portion (m. 157° from Et<sub>2</sub>O) remained unsatd. toward KMnO<sub>4</sub>, but was apparently not identical with VIII and remained unchanged on heating with aqueous H<sub>2</sub>SO<sub>4</sub>. The only hydrogenated portion obtained from VIII was converted through its acid chloride into 2-PhNHCOC<sub>6</sub>H<sub>10</sub>CH<sub>2</sub>CH<sub>2</sub>CONHPh, m. 212° (cf. Huckel, C.A. 19, 1269). III was a mixture of 75% mono- and 25% dibasic acids, which with concentrated H<sub>2</sub>SO<sub>4</sub> gave IV. Catalytic hydrogenation of III gave small amts. of V and a brown oil, which when refluxed 24 hrs. with 40% KOH, diluted, and oxidize with 5% KMnO<sub>4</sub>, yielded about 10% 1,2-(HO<sub>2</sub>C)2C<sub>6</sub>H<sub>10</sub>. III with CH<sub>2</sub>N<sub>2</sub> gave a mixture, of which the fraction b<sub>12</sub> 175-90° gave on saponification VIII and a compound m. 211° (yielding a hydrogenation product, m. 188°, not identical with VI); another fraction, b<sub>12</sub> 190-210°, when saponified gave small amts. of VIII.

L8 ANSWER 31 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN

TI 2,4-Pentadienoic acids

AN 1950:52175 CAPLUS

DN 44:52175

OREF 44:9979b-d

TI 2,4-Pentadienoic acids

IN Geyer, Bradford P.; Ballard, Seaver A.

PA Shell Development Co.

DT Patent

LA Unavailable

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 2515595		19500718	US 1948-39817	19480720
AB	A 2,4-pentadienoic acid is produced by the liquid-phase condensation of an α-methylenealkanal with CH <sub>2</sub> :CO (I) in the presence of a basic catalyst. Thus, into CH <sub>2</sub> :CHCHO (II) 84 g. (containing 0.1% p-(HO)2C <sub>6</sub> H <sub>4</sub> and				

NaOAc 10 g. in Et<sub>2</sub>O 200 cc. at -30° is passed I (more than 52 g. in 4 hrs.), the mixture filtered, the filtrate distilled to remove II and Me<sub>2</sub>CO, the residue (128 g.) neutralized at 0° with aqueous NaOH, 300 cc. HCCl<sub>3</sub> added, the mixture acidified with 25% HCl at 0°, the HCCl<sub>3</sub> layer dried and distilled at 0.2 mm., and CH<sub>2</sub>:CHCH:CHCO<sub>2</sub>H, m. 71°, isolated by sublimation.

L8 ANSWER 32 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN

TI Butadienyl compounds

AN 1937:25080 CAPLUS

DN 31:25080

OREF 31:3503h-i,3504a-c

TI Butadienyl compounds

IN Carothers, Wallace H.; Berchet, Gerard J.

PA E. I. du Pont de Nemours & Co.

DT Patent

LA Unavailable

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 2073363		19370309	US 1932-640326	19321029
AB	4-Hydroxy-1,2-butadiene may be formed by heating 4-chloro-1,2-butadiene with an oxide or carbonate such as CaO or Na <sub>2</sub> CO <sub>3</sub> in water at 60-90° for 15 hrs.; by fractional distillation, a purified product is obtained which				

is

a colorless liquid b756 126-8° which has a powerful vesicant action on the skin and the vapor of which has a strongly irritating effect upon the mucous membranes. It tends to polymerize when heated. By reaction with Me<sub>2</sub>SO<sub>4</sub>, etc., alkyl ethers of the hydroxy-1,2-butadiene are formed, and aromatic ethers are formed from it by reaction with metallic phenolates. Details are also given of the production of 4-phenoxy-1,2-butadiene, esters such as the formic, acetic, trichloroacetic, succinic, benzoic, phthalic and p-nitrobenzoic esters, the chlorocarbonic ester, b57 66-8° and suitable for use in the preparation of urethans having medicinal properties or the production of different esters by reaction with an alc. or a phenol, and of the production of butadienyl thiocyanate, butadienyl chloride, butadienyl cyanide, β,δ-dimethoxyvaleronitrile, polymerized butadienyl cyanide, ethyl β-vinyl acrylate (which polymerizes to a rubber-like mass on heating to 100° for 10 hrs.), β-vinylacrylic acid and a polymer, various amines of 4-hydroxy-1,2-butadiene, α-N-naphthyl-N'-2,3-butadienyl-1-urea, m. 77°, di- and tri-(2,3-butadienyl)amines, mono(2,3-butadienyl)aniline, di(2,3-butadienyl)aniline, butadienylacetic acid, butadienylacetone, ethylbutadienylbarbituric acid, isomers and dehydration products of 4-hydroxy-1,2-butadiene, methyl, ethyl, butyl, heptyl, butadienyl and phenylethyl esters of butadienylacetic and of methylethenylpropionic acids, butadienyl mercaptan and butadienyl sulfide, phenyl-p-tolylbutadienylcarbinol, etc. The butadienylamines may be used for the manufacture of dyes and pharmaceutical chemicals and for inhibiting oxidation of substances such as rubber and natural unsatd. fatty oils. Numerous details of procedure and properties of the products obtained are given.

L8 ANSWER 33 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN

TI A hypothesis on the biological origin of resin acids

AN 1925:26895 CAPLUS

DN 19:26895

OREF 19:3485f-h

TI A hypothesis on the biological origin of resin acids

AU Aschan, Ossian

SO Chemiker-Zeitung (1925), 49, 689-91

CODEN: CMKZAT; ISSN: 0009-2894

DT Journal

LA Unavailable  
 AB cf. C. A. 15, 3096; 17, 1228; 18, 2151. The formulas of terpenes, polyterpenes and resin acids are all multiples of isoprene, C<sub>5</sub>H<sub>8</sub>. Their formation from this common building stone by the action of enzymes appears more probable than the formation of resin acids by oxidation of terpenes. The rubber production by tropical plants and the presence of isoprene, isoamylene and isopentane in masut suggest that isoprene is a widely spread plant metabolite in all latitudes as well as in the prehistoric epoch. The following is the hypothetical formation of isoprene (I) and vinylacrylic acid (II) from the normal intermediates of enzymic carbohydrate decomposition: Acetone, dihydroxyacetone and pyruvic acid condense with AcH to aldols, which after their reduction to the glycols split off water. The condensation of 2-4 mols. I leads to all the mono- and diterpenes of the Pinus species (abietin, pinabietin, colophene). The condensation of 3 mols. I with 1 mol. II yields a hypothetical abietic acid, the structure of which resembles closely that of Virtannen's pinabietic acids.

=> d his

(FILE 'HOME' ENTERED AT 06:07:53 ON 11 DEC 2007)

FILE 'REGISTRY' ENTERED AT 06:08:12 ON 11 DEC 2007  
 L1 0 2,4-PENTADIENEOIC ACID/CN  
 E 2,4-PENTADIENEOIC ACID/CN  
 E 2,4-PENTADIENEOIC ACID/CN  
 E 2,4-PENTADIENEOIC ACID, 5-METHYL/CN  
 L2 STRUCTURE UPLOADED  
 L3 0 SEARCH L2 EXACT SAM  
 L4 3 SEARCH L2 EXACT FULL

FILE 'CAPLUS' ENTERED AT 06:16:55 ON 11 DEC 2007  
 L5 9 L4

FILE 'REGISTRY' ENTERED AT 06:27:46 ON 11 DEC 2007

FILE 'CAPLUS' ENTERED AT 06:28:11 ON 11 DEC 2007

FILE 'REGISTRY' ENTERED AT 06:29:04 ON 11 DEC 2007  
 E 2,4-PENTADIENEOIC ACID/CN  
 L6 1 E3

FILE 'CAPLUS' ENTERED AT 06:29:37 ON 11 DEC 2007  
 L7 2 L6/THU

FILE 'REGISTRY' ENTERED AT 06:32:17 ON 11 DEC 2007

FILE 'CAPLUS' ENTERED AT 06:32:27 ON 11 DEC 2007  
 L8 33 L6/PREP

=> file reg

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DICTIONARY FILE UPDATES: 10 DEC 2007 HIGHEST RN 957336-90-2

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<http://www.cas.org/support/stngen/stndoc/properties.html>

=> e 5-phenyl- 2,4-pentadienoic acid/cn

E1	1	5-PHENYL MELDRUM'S ACID/CN
E2	1	5-PHENYL(1,3,4)OXADIAZOLE-2-CARBONYL CHLORIDE/CN
E3	0 -->	5-PHENYL- 2,4-PENTADIENOIC ACID/CN
E4	1	5-PHENYL-(1,3,4)OXADIAZOLE-2-CARBOXYLIC ACID (4-FLUORO-3-(PYRAZIN-2-YLOXYMETHYL) PHENYL)AMIDE/CN
E5	1	5-PHENYL-(1,3,4)OXADIAZOLE-2-CARBOXYLIC ACID N-(5-(BENZOYL(METHYL)AMINO)-1-(2-CARBAMOYLETHYL)-1H-BENZIMIDAZOL-2-YL)AMIDE/CN
E6	1	5-PHENYL-(2E,4E)-PENTADIENOYL CHLORIDE/CN
E7	1	5-PHENYL-(3S)-HYDROXY-1-PENTYNE/CN
E8	1	5-PHENYL-1,10-PHENANTHROLINE/CN
E9	1	5-PHENYL-1,2,3,4-TETRAZOLE/CN
E10	1	5-PHENYL-1,2,3,4-THIATRIAZOLE/CN
E11	1	5-PHENYL-1,2,3,4-THIATRIAZOLE-3-OXIDE/CN
E12	1	5-PHENYL-1,2,3-THIADIAZOLE/CN

=> e 2,4-pentadienoic acid, 5-phenyl/cn

E1	1	2,4-PENTADIENOIC ACID, 5-PHENOXY-, ETHYL ESTER/CN
E2	1	2,4-PENTADIENOIC ACID, 5-PHENOXY-, METHYL ESTER/CN
E3	0 -->	2,4-PENTADIENOIC ACID, 5-PHENYL/CN
E4	2	2,4-PENTADIENOIC ACID, 5-PHENYL-/CN
E5	1	2,4-PENTADIENOIC ACID, 5-PHENYL-, ((2-METHYL-1-OXO-2-PROPENYL)OXY)METHYL ESTER/CN
E6	1	2,4-PENTADIENOIC ACID, 5-PHENYL-, ((2-METHYL-1-OXO-2-PROPENYL)OXY)METHYL ESTER, POLYMER WITH BUTYL 2-METHYL-2-PROPENOATE AND 2-METHYL-2-PROPENOIC ACID/CN
E7	1	2,4-PENTADIENOIC ACID, 5-PHENYL-, (2,2'-BIPYRIDINE)-4,4'-DIYLBIS(METHYLENE) ESTER, (2E,2'E,4E,4'E)-/CN
E8	1	2,4-PENTADIENOIC ACID, 5-PHENYL-, (2,4,6-TRIOXO-1,3,5-TRIAZINE-1,3,5(2H,4H,6H)-TRIYL)TRI-2,1-ETHANEDIYL ESTER/CN
E9	1	2,4-PENTADIENOIC ACID, 5-PHENYL-, (2,4-DICHLOROPHENYL) (DIETHOXYPHOSPHINYL)METHYL ESTER, (2E,4E)-/CN
E10	1	2,4-PENTADIENOIC ACID, 5-PHENYL-, (2-CHLOROPHENYL) (DIETHOXYPHOSPHINYL)METHYL ESTER, (2E,4E)-/CN
E11	1	2,4-PENTADIENOIC ACID, 5-PHENYL-, (2E)-4-ETHOXY-4-OXO-2-BUTEN-1-YL ESTER, (2E,4E)-/CN
E12	1	2,4-PENTADIENOIC ACID, 5-PHENYL-, (2E,4E)-/CN

=> e4

L9 2 "2,4-PENTADIENOIC ACID, 5-PHENYL-"/CN



=> d 19

L9 ANSWER 1 OF 2 REGISTRY COPYRIGHT 2007 ACS on STN  
RN 54352-97-5 REGISTRY  
ED Entered STN: 16 Nov 1984  
CN 2,4-Pentadienoic acid, 5-phenyl- (9CI) (CA INDEX NAME)  
OTHER NAMES:  
CN Juarezic acid  
MF C11 H10 O2  
LC STN Files: BEILSTEIN\*, CA, CAPLUS, CHEMINFORMRX, IFICDB, IFIUDB  
(\*File contains numerically searchable property data)

Ph-CH=CH-CH=CH-CO<sub>2</sub>H

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1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> file caplus

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CA SUBSCRIBER PRICE	0.00	-6.24

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=> 19

L10 158 L9

=> 9/thu

0 9/CT  
960327 THU/RL

L11 0 9/THU  
(9/CT (L) THU/RL)

=> 19/thu

158 L9  
960327 THU/RL  
L12 10 L9/THU  
(L9 (L) THU/RL)

=> d 112 1-10 ti

L12 ANSWER 1 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN  
TI Prosthetic implant materials containing donepezil, and artificial tissue containing the same

L12 ANSWER 2 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN  
TI Method for manufacturing tissue body with implant materials containing donepezil, and implant materials

L12 ANSWER 3 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN  
TI Visible light-curable materials and their use for wound healing promoters

L12 ANSWER 4 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN  
TI Physiologically active substance-coated stents, their manufacture, and sustained-release drug delivery using them

L12 ANSWER 5 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN  
TI Energy properties of statistical copolymer thin films as a measure of their biocompatibility with oncological medicine

L12 ANSWER 6 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN  
TI The novel histone deacetylase inhibitor BL1521 inhibits proliferation and induces apoptosis in neuroblastoma cells

L12 ANSWER 7 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN  
TI Induction of histone acetylation and inhibition of growth by phenyl alkanoic acids and structurally related molecules

L12 ANSWER 8 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN  
TI Preparation of arylalkanoic acids and hydroxamic acids as histone deacetylase inhibitors for treatment of cancer, hematological disorders, and genetic related metabolic disorders

L12 ANSWER 9 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN  
TI Preparation of arylalkanoic acids and hydroxamic acids as histone deacetylase inhibitors for treatment of cancer, hematological disorders, and genetic related metabolic disorders

L12 ANSWER 10 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN  
TI Structure-antibacterial activity relationship of some aromatic acids

=> d 112 6-10 ti fbib abs

L12 ANSWER 6 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN  
TI The novel histone deacetylase inhibitor BL1521 inhibits proliferation and induces apoptosis in neuroblastoma cells  
AN 2004:733540 CAPLUS  
DN 141:325331  
TI The novel histone deacetylase inhibitor BL1521 inhibits proliferation and induces apoptosis in neuroblastoma cells  
AU de Ruijter, Annemieke J. M.; Kemp, Stephan; Kramer, Gertjan; Meinsma, Rutger J.; Kaufmann, Judith O.; Caron, Huib N.; van Kuilenburg, Andre B.

P.  
 CS Laboratory Genetic Metabolic Diseases, Department of Paediatrics/Emma Children's Hospital and Clinical Chemistry, Academic Medical Centre, University of Amsterdam, Amsterdam, 1100 DE, Neth.  
 SO Biochemical Pharmacology (2004), 68(7), 1279-1288  
 CODEN: BCPA6; ISSN: 0006-2952  
 PB Elsevier B.V.  
 DT Journal  
 LA English  
 AB Neuroblastoma is a childhood cancer arising from the sympathetic nervous system. Disseminated neuroblastoma has a poor prognosis despite intensive multimodality treatment. Histone deacetylases (HDACs) were recently discovered as a potential target for pharmacol. gene therapy in cancer. HDACs have an important function in regulating DNA packaging in chromatin, thereby affecting the transcription of genes. In this paper, we tested the efficacy of a newly developed histone deacetylase inhibitor, BL1521, on neuroblastoma in vitro by investigating the changes in: acetylation of histone H3, in situ HDAC activity, p21WAF1/CIP1 and MYCN expression, metabolic activity, proliferation, morphol. and the amount of apoptosis present. BL1521 inhibited the in situ HDAC activity of a panel of neuroblastoma cell lines by at least 85%. Western anal. showed an increase of histone H3 acetylation in neuroblastoma cells after incubation with BL1521. Northern anal. showed an increase in the expression of p21WAF1/CIP1 and a decrease in the expression of MYCN in neuroblastoma cells after incubation with BL1521. Proliferation as well as the metabolic activity of neuroblastoma cells decreased significantly in response to treatment with BL1521, regardless of the MYCN status of the cells. BL1521 induced poly-(ADP-ribose) polymerase cleavage in a time- and dose-dependent manner, indicating the induction of apoptosis. Furthermore, when compared to the HDAC inhibitors Trichostatin A and 4-phenylbutyrate, BL1521 has an intermediate efficacy. Our results show that BL1521 is a potent inhibitor of HDAC and that HDACs are an attractive target for selective chemotherapy in neuroblastoma.

RE.CNT 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD  
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 7 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN  
 TI Induction of histone acetylation and inhibition of growth by phenyl alkanolic acids and structurally related molecules  
 AN 2004:450167 CAPLUS  
 DN 142:32394  
 TI Induction of histone acetylation and inhibition of growth by phenyl alkanolic acids and structurally related molecules  
 AU Lea, Michael A.; Shareef, Asif; Sura, Monali; desBordes, Charles  
 CS Department of Biochemistry and Molecular Biology, UMDNJ-New Jersey Medical School, Newark, NJ, 07103, USA  
 SO Cancer Chemotherapy and Pharmacology (2004), 54(1), 57-63  
 CODEN: CCPHDZ; ISSN: 0344-5704  
 PB Springer-Verlag  
 DT Journal  
 LA English  
 AB Purpose. A structure-activity study was undertaken to determine the influence of side chain length of Ph alkanolic acids and the degree of unsatn. of Ph alkenolic acids on the induction of histone acetylation and inhibition of cancer cell proliferation. Materials and methods. Studies on cell proliferation were performed with DS19 mouse erythroleukemic cells, PC-3 human prostate cancer cells and Caco-2 human colon cancer cells. Actions on histone deacetylase and the induction of histone acetylation were compared for 4-phenylbutyrate and structurally related mols. Results. Increasing inhibition of cell proliferation by Ph alkanolic acids together with a decrease in cells in S phase and an increase in apoptotic cells was observed with increased chain length between four and ten carbons. Introduction of double bonds into the side chain was associated with

increased growth inhibition. In contrast, 4-phenylbutyrate was a more potent inhibitor of histone deacetylase and inducer of histone acetylation than the other Ph alkanolic acids examined. Conclusions. In comparison with the action of 4-phenylbutyrate, actions other than inhibition of histone deacetylase appear to be more important for growth inhibition by longer chain Ph alkanolic and Ph alkenolic acids.

RE.CNT 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 8 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN

TI Preparation of arylalkanoic acids and hydroxamic acids as histone deacetylase inhibitors for treatment of cancer, hematological disorders, and genetic related metabolic disorders

AN 2002:755220 CAPLUS

DN 137:262850

TI Preparation of arylalkanoic acids and hydroxamic acids as histone deacetylase inhibitors for treatment of cancer, hematological disorders, and genetic related metabolic disorders

IN Lan-Hargest, Hsuan-yin; Kaufman, Robert J.; Wiech, Norbert L.

PA USA

SO U.S. Pat. Appl. Publ., 19 pp.

CODEN: USXXCO

DT Patent

LA English

FAN.CNT 8

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WO	2002076941	A3	20040212		
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PATENT FAMILY INFORMATION:

FAN 2002:754352

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FAN	2002:755255				
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US 2004029922	A1	20040212	WO 2003-US15839	W	20030521
US 7057057	B2	20060606	US 2003-442177		20030521
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FAN 2003:950999					
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FAN 2004:453179

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WO 2004046104	A3	20040805		
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FAN 2004:701812

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US 2002143037	A1	20021003	US 2002-427567P	P 20021120
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			US 2001-812940	B1 20010327

OS MARPAT 137:262850

AB Title compds. AY1LY2C(:X1)X2 (I) [wherein A = (un)substituted (hetero)cycloalkyl, (hetero)cycloalkenyl, (hetero)aryl; or A =



(un)substituted hydrocarbon chain interrupted by O, S, NRa, CO, NRaSO<sub>2</sub>, SO<sub>2</sub>NRa, NRaCO<sub>2</sub>, OCONRa, NRaCONRb, OCO, CO<sub>2</sub>, OSO<sub>2</sub>, SO<sub>2</sub>O, or OCO<sub>2</sub>; Y1 and Y2 = independently CH<sub>2</sub>, O, S, NRc, NRcCO<sub>2</sub>, OCONRc, NRcCONRd, OCO<sub>2</sub>, or a bond; Ra, Rb, Rc, and Rd = independently H, (hydroxy)alkyl, alkenyl, alkynyl, alkoxy, OH, or haloalkyl; L = (un)substituted straight hydrocarbon chain optionally containing at least one double and/or triple bond; X1 = O or S; X2 = OR1, SR1, NR3OR1, NR3SR1, CO<sub>2</sub>R1, CHR4OR1, N:NCON(R3)2, or OCHR4OCOR5; R1 and R2 = independently H, (hydroxy)alkyl, haloalkyl, or hydroxy protecting group; R3 = H, (hydroxy)alkyl, alkenyl, alkynyl, alkoxy, OH, haloalkyl, or amino protecting group; R4 = OH, (hydroxy)alkyl, or haloalkyl; R5 = (hydroxy)alkyl or haloalkyl; provided that when L = Et or Pr and X2 = OR1, then Y1 ≠ a bond and Y2 ≠ a bond; or salts thereof] where prepared with Zn-binding moieties, such as hydroxamic acid or carboxylic acid groups, for inhibiting histone deacetylation activity in cells. For example, Et (trans)-cinnamate was treated with MeMgI in anhydrous ether to give 4-phenyl-2-methyl-3-buten-2-ol, which was converted to 3-methyl-5-phenyl-2,4-pentadienal using PO<sub>3</sub>Cl in DMF. Oxidation of the aldehyde with aqueous AgNO<sub>3</sub> in EtOH afforded the desired 3-methyl-5-phenyl-2,4-pentadienoic acid (II). Test compds. of the invention showed potent inhibition of histone deacetylase with IC<sub>50</sub> values in the low μM range; e.g. two test compds. showed IC<sub>50</sub> values of 1.7 μM and 1.9 μM. Histone deacetylase inhibition can repress gene expression, including expression of genes related to tumor suppression. Thus, I provide an alternate route for treating cancer, hematol. disorders, e.g., hemoglobinopathies, and genetic related metabolic disorders, e.g., cystic fibrosis and adrenoleukodystrophy (no data).

L12 ANSWER 9 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN

TI Preparation of arylalkanoic acids and hydroxamic acids as histone deacetylase inhibitors for treatment of cancer, hematological disorders, and genetic related metabolic disorders

AN 2002:754352 CAPLUS

DN 137:262849

TI Preparation of arylalkanoic acids and hydroxamic acids as histone deacetylase inhibitors for treatment of cancer, hematological disorders, and genetic related metabolic disorders

IN Lan-Hargest, Hsuan-Yin; Kaufman, Robert J.; Wiech, Nobert L.

PA Circagen Pharmaceutical, USA

SO PCT Int. Appl., 66 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 8

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				US 2001-25947	A1 20011226
	US 2002143196	A1	20021003	US 2001-812944	20010327
	US 6495719	B2	20021217		

US 2002143052	A1	20021003	US 2001-812945	20010327
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			US 2001-25947	A 20011226
			WO 2002-US8836	W 20020325
AU 2002250401	A1	20021008	AU 2002-250401	20020325
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			US 2001-812945	A 20010327
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EP 1408946	A2	20040421	EP 2002-719311	20020325
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			WO 2002-US8836	W 20020325

PATENT FAMILY INFORMATION:

FAN 2002:755220

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	CA 2442366	A1	20021003	CA 2002-2442366	20020325
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			US 2001-25947	A 20011226	

US 2003125306	A1	20030703	WO 2002-US8836	W	20020325
			US 2002-318225		20021213
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US 2005171208	A1	20050804	US 2001-812945	A3	20010327
			US 2005-59377		20050217
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			US 2006-489519		20060720
			US 2001-812944	A3	20010327
			US 2001-812945	A2	20010327
			US 2002-382075P	P	20020522
			US 2002-382077P	P	20020522
			US 2002-382089P	P	20020522
			US 2003-442175	A1	20030521
			US 2003-442177	A3	20030521
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US 2002-382089P	P 20020522
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US 2003-442177	A3 20030521
US 2003-442191	A1 20030521
US 2005-59377	A2 20050217
US 2005-198293	A1 20050808

FAN 2003:950833

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WO 2003099272	A1	20031204	WO 2003-US15839	20030521
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AU 2003243272	A1	20031212	WO 2003-US15839	W 20030521
			AU 2003-243272	20030521
			US 2002-382089P	P 20020522
US 2004029922	A1	20040212	WO 2003-US15839	W 20030521
US 7057057	B2	20060606	US 2003-442177	20030521
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EP 1511477	A1	20050309	EP 2003-755395	20030521
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US 2005282890	A1	20051222	WO 2003-US15839	W 20030521
			US 2005-198293	20050808
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			US 2003-442177	A3 20030521

FAN 2003:950971

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WO 2003099760	A1	20031204	WO 2003-US15996	20030521
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			US 2002-382075P	P 20020522
US 2004029903	A1	20040212	WO 2003-US15996	W 20030521
			US 2003-442175	20030521

US 7193105	B2	20070320	US 2002-382075P	P	20020522
EP 1511715	A1	20050309	EP 2003-755410		20030521
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FAN 2003:950999					
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			WO 2003-US36981	W	20031119
AU 2003291097	A1	20040615	AU 2003-291097		20031119
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IN 2005DN02110	A	20070119	IN 2005-DN2110	20050518
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				US 2001-812940	B1 20010327

OS MARPAT 137:262849

AB Title compds. AY1LY2C(:X1)X2 (I) [wherein A = (un)substituted (hetero)cycloalkyl, (hetero)cycloalkenyl, (hetero)aryl; or A = (un)substituted hydrocarbon chain interrupted by O, S, NRa, CO, NRaSO2, SO2NRa, NRaCO2, OCONRa, NRaCONRb, OCO, CO2, OSO2, SO2O, or OCO2; Y1 and Y2 = independently CH2, O, S, NRc, NRcCO2, OCONRc, NRcCONRd, OCO2, or a bond; Ra, Rb, Rc, and Rd = independently H, (hydroxy)alkyl, alkenyl, alkynyl, alkoxy, OH, or haloalkyl; L = (un)substituted straight hydrocarbon chain optionally containing at least one double and/or triple bond; X1 = O or S; X2 = OR1, SR1, NR3OR1, NR3SR1, CO2R1, CHR4OR1, N:NCON(R3)2, or OCHR4OCOR5; R1 and R2 = independently H, (hydroxy)alkyl, haloalkyl, or hydroxy protecting group; R3 = H, (hydroxy)alkyl, alkenyl, alkynyl, alkoxy, OH, haloalkyl, or amino protecting group; R4 = OH, (hydroxy)alkyl, or haloalkyl; R5 = (hydroxy)alkyl or haloalkyl; provided that when L = Et or Pr and X2 = OR1, then Y1 ≠ a bond and Y2 ≠ a bond; or salts thereof] where prepared with Zn-binding moieties, such as hydroxamic acid or carboxylic acid groups, for inhibiting histone deacetylation activity in cells. For example, Et (trans)-cinnamate was treated with MeMgI in anhydrous ether to give 4-phenyl-2-methyl-3-buten-2-ol, which was converted to 3-methyl-5-phenyl-2,4-pentadienal using PO3Cl in DMF. Oxidation of the aldehyde with aqueous AgNO3 in EtOH afforded the desired 3-methyl-5-phenyl-2,4-pentadienoic acid (II). Test compds. of the invention showed potent inhibition of histone deacetylase with IC50 values in the low μM range; e.g. two test compds. showed IC50 values of 1.7 μM and 1.9 μM. Histone deacetylase inhibition can repress gene expression, including expression of genes related to tumor suppression. Thus, I provide an alternate route for treating cancer, hematol. disorders, e.g., hemoglobinopathies, and genetic related metabolic disorders, e.g., cystic fibrosis and adrenoleukodystrophy (no data).

L12 ANSWER 10 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN

TI Structure-antibacterial activity relationship of some aromatic acids

AN 1998:797015 CAPLUS

DN 130:194161

TI Structure-antibacterial activity relationship of some aromatic acids

AU Abeytunga, D. T. U.; Peiris, T. E. M.; Wijesundera, R. L. C.

CS Department of Chemistry, University of Colombo, Colombo, 3, Sri Lanka

SO Journal of the National Science Council of Sri Lanka (1998), 26(2), 133-139

CODEN: JNSCBH; ISSN: 0300-9254

PB Natural Resources, Energy and Science Authority of Sri Lanka

DT Journal

LA English

AB Nine aromatic acids were tested for their antibacterial effect against Staphylococcus aureus. 3-Phenylpropanoic acid was identified as the most active of the acids chosen for this bioassay. In general a 3,4-methylenedioxy substituent on the Ph group reduces the activity against Staphylococcus aureus.

RE.CNT 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> 110/prep

FIELD CODES CANNOT BE CHANGED HERE

You may have tried to apply a field code to a term that already has a field code. You can only add a field code to a term that has no field code appended to it.

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(FILE 'HOME' ENTERED AT 06:07:53 ON 11 DEC 2007)

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E 2,4-PENTADIENOIC ACID/CN  
E 2,4-PENTADIENOIC ACID/CN  
E 2,4-PENTADIENOIC ACID, 5-METHYL/CN  
L2 STRUCTURE UPLOADED  
L3 0 SEARCH L2 EXACT SAM  
L4 3 SEARCH L2 EXACT FULL

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L5 9 L4

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1 E3

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L8 33 L6/PREP

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L9 E 5-PHENYL- 2,4-PENTADIENOIC ACID/CN  
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2 E4

FILE 'CAPLUS' ENTERED AT 06:39:43 ON 11 DEC 2007

L10 158 L9  
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L12 10 L9/THU

=> 19/prep

158 L9  
4500485 PREP/RL  
L13 52 L9/PREP  
(L9 (L) PREP/RL)

=> 113 not 112

L14 49 L13 NOT L12

=> d 114 39-49 ti

L14 ANSWER 39 OF 49 CAPLUS COPYRIGHT 2007 ACS on STN  
 TI The mechanism of the reaction of bromine with 2,2-diphenylpenten-4-oic acid and its esters

L14 ANSWER 40 OF 49 CAPLUS COPYRIGHT 2007 ACS on STN  
 TI Reduction of unsaturated acid amides to unsaturated aldehydes; a contribution to the synthesis of polyene chains

L14 ANSWER 41 OF 49 CAPLUS COPYRIGHT 2007 ACS on STN  
 TI Diene syntheses. XXIX. Diene syntheses with unsymmetrical addends; the 1,4-disubstituted diene type

L14 ANSWER 42 OF 49 CAPLUS COPYRIGHT 2007 ACS on STN  
 TI Unsaturated organic compounds

L14 ANSWER 43 OF 49 CAPLUS COPYRIGHT 2007 ACS on STN  
 TI Condensation of aldehydes with malonic acid. XIX. Condensation of cinnamaldehyde

L14 ANSWER 44 OF 49 CAPLUS COPYRIGHT 2007 ACS on STN  
 TI Synthesis of some 5-substituted 5-hydroxy-2-pentenoic acids

L14 ANSWER 45 OF 49 CAPLUS COPYRIGHT 2007 ACS on STN  
 TI Reformatsky condensations involving vinyls of haloacetic esters

L14 ANSWER 46 OF 49 CAPLUS COPYRIGHT 2007 ACS on STN  
 TI o-Methoxyphenylmalonic acid and its derivatives

L14 ANSWER 47 OF 49 CAPLUS COPYRIGHT 2007 ACS on STN  
 TI General synthesis of  $\alpha$ -unsaturated acids from malonic acid

L14 ANSWER 48 OF 49 CAPLUS COPYRIGHT 2007 ACS on STN  
 TI Polymerization of allyl cinnamalacetate

L14 ANSWER 49 OF 49 CAPLUS COPYRIGHT 2007 ACS on STN  
 TI The distillation products of  $\alpha$ -truxilic acid. Obtainment of a fourth truxillic acid

=> d 114 39,40, 41, 47-49 ti fbib abs

L14 ANSWER 39 OF 49 CAPLUS COPYRIGHT 2007 ACS on STN  
 TI The mechanism of the reaction of bromine with 2,2-diphenylpenten-4-oic acid and its esters  
 AN 1953:18972 CAPLUS  
 DN 47:18972  
 OREF 47:3271d-e  
 TI The mechanism of the reaction of bromine with 2,2-diphenylpenten-4-oic acid and its esters  
 AU Lindsay, Kenneth L.  
 CS Univ. of Minnesota, Minneapolis  
 SO (1952) 92 pp. Avail.: Univ. Microfilms (Ann Arbor, Mich.), Order No. 4341  
 From: Dissertation Abstracts 12, 814-15  
 DT Dissertation  
 LA Unavailable  
 AB Unavailable

L14 ANSWER 40 OF 49 CAPLUS COPYRIGHT 2007 ACS on STN  
 TI Reduction of unsaturated acid amides to unsaturated aldehydes; a contribution to the synthesis of polyene chains  
 AN 1953:18971 CAPLUS  
 DN 47:18971  
 OREF 47:3270c-i,3271a-d



TI Reduction of unsaturated acid amides to unsaturated aldehydes; a contribution to the synthesis of polyene chains  
 AU Wittig, Georg; Hornberger, Paul  
 CS Univ. Tübingen, Germany  
 SO Ann. (1952), 577, 11-25  
 DT Journal  
 LA Unavailable  
 OS CASREACT 47:18971  
 AB Mixed at  $-78^{\circ}$  and then heated 24 hrs. at  $125^{\circ}$  in a sealed tube (or autoclave), 2.7 g. LiH and 7.1 g.  $\text{BF}_3 \cdot \text{Et}_2\text{O}$  in absolute  $\text{Et}_2\text{O}$  gave 4 g.  $\text{LiBH}_4 \cdot \text{Et}_2\text{O}$  (I), extremely hygroscopic, forming a solution without decomposing. Heated at  $33^{\circ}$ , I lost  $\text{Et}_2\text{O}$ , giving  $\text{LiBH}_4$ , m.  $278-9^{\circ}$ , exploding when heated in a free flame. Similarly formed from NaH was  $\text{NaBH}_4$ , insol. in  $\text{Et}_2\text{O}$ , soluble in iso- $\text{PrNH}_2$ . Heated under N at  $175^{\circ}$ , 11.5 g.  $\text{B}(\text{O}i\text{Bu})_3$  (II) and 0.4 g. LiH, followed by  $\text{Et}_2\text{O}$  addition, gave 10 g.  $\text{Li}[\text{BH}(\text{O}i\text{Bu})_3] \cdot 0.5\text{Et}_2\text{O}$  (III), rectangles, decomposing in air, yielding H with  $\text{H}_2\text{O}$  or alc., soluble in tetrahydrofuran (IIIa), slightly soluble in  $\text{Et}_2\text{O}$  and  $\text{C}_6\text{H}_6$ , practically insol. in dioxane. II heated with excess LiH gave I. Techniques for analyzing the various Li derivs. are outlined.  $\text{Ph}_2\text{Zn}$  (2.2 g.) and 0.8 g. LiH warmed to  $90^{\circ}$ , treated with  $\text{Et}_2\text{O}$ , and "dried" over paraffin gave 2.5 g.  $\text{Li}[\text{ZnHPh}_2] \cdot \text{Et}_2\text{O}$ , having solubilities similar to those of III.  $\text{Ph}_2\text{Be}$  from  $\text{Ph}_2\text{Hg}$  (cf. C.A. 45, 5556b) was freed from xylene by distillation under N, taken up in  $\text{Et}_2\text{O}$ , and separated from  $\text{BeHg}$ , giving  $\text{Ph}_2\text{Be} \cdot 2\text{Et}_2\text{O}$  (IV), cubes, m.  $28-32^{\circ}$ , losing  $\text{Et}_2\text{O}$  when heated in vacuo at  $130^{\circ}$ . IV (3.1 g.) and 0.8 g. LiH under N at  $160-5^{\circ}$ , followed by  $\text{Et}_2\text{O}$  extraction, gave  $\text{Li}(\text{BeHPh}_2) \cdot \text{Et}_2\text{O}$ , rhombs (stored under N), decomposing in air with evolution of heat and light, giving H on treatment with  $\text{H}_2\text{O}$ .  $\text{PhCH:CHCOCl}$  (V) (8.4 g.) and  $\text{Ph}_2\text{NH}$  in absolute  $\text{Et}_2\text{O}$  gave 13.3 g.  $\text{PhCH:CHCONPh}_2$  (VI), m.  $152-3^{\circ}$ . VI (3 g.) suspended in 15 cc. dry  $\text{Et}_2\text{O}$ , heated 1 hr. with M I, and treated with aqueous HCl was not reduced, but gave 90% of a stereoisomeric or polymorphic modification (VII) of VI, leaflets, m.  $191-2^{\circ}$ , which, when inoculated at  $130^{\circ}$  with VI, gave the latter. However molten VI was not converted into VII by inoculation. VII was also obtained by heating VI with  $\text{LiAlH}_4$  (VIII) in IIIa or  $\text{Et}_2\text{O}$ , unless a large excess VIII was used, whereupon VII was no longer formed, but 37%  $\text{PhCH:CHCH}_2\text{OH}$ , b.p.  $135-8^{\circ}$  (phenylurethan, m.  $89-91^{\circ}$ ), was obtained (in the  $\text{Et}_2\text{O}$  extract). V (18.3 g.) and 16.7 g. carbazole (IX), stirred 0.5 hr. at  $200^{\circ}$ , cooled, triturated with 100 cc. MeOH, and cooled to  $0^{\circ}$ , gave 21 g. 9-cinnamoyl derivative (X) of IX, m.  $96-6.5^{\circ}$ . With VIII, X in  $\text{Et}_2\text{O}$  at  $0^{\circ}$ , followed by addition of  $\text{PhNHNH}_2$ , gave a mixture of 2.55 g.  $\text{PhCH:CHCH:NNHPh}$ , m.  $166-7^{\circ}$ , and IX (subliming from the mixture at 0.1 mm. and  $120^{\circ}$ ).  $\text{Ph}(\text{CH:CH})_2\text{COCl}$  in absolute  $\text{Et}_2\text{O}$  and  $\text{Me}_2\text{NH} \cdot \text{HCl}$ , treated dropwise with concentrated aqueous KOH, gave 88%  $\text{Ph}(\text{CH:CH})_2\text{CONMe}_2$  (XI), m.  $109-10^{\circ}$  (from  $\text{C}_6\text{H}_6$ -petr. ether). XI was not reduced by I or VIII, but with VIII gave an unstable isomer of XI (cis-trans?), m.  $70-2^{\circ}$  (from cyclohexane in the dark), reconverted into XI on standing or on repeated crystallization.  $\text{Ph}(\text{CH:CH})_2\text{COCl}$  (9.6 g.) heated with 8.4 g. IX in xylene gave 10.1 g. 9- $\text{Ph}(\text{CH:CH})_2\text{CO}$  derivative (XII) of IX, lemon-yellow leaflets, m.  $124-5^{\circ}$ . I heated with XII in  $\text{Et}_2\text{O}$ , followed by addition of aqueous HCl, gave 62%  $\text{Ph}(\text{CH:CH})_2\text{CHO}$  (phenylhydrazone, m.  $177-9^{\circ}$ ), also formed in 72.9% yield by heating XII with VIII.  $\text{Ph}(\text{CH:CH})_3\text{CHO}$ , m.  $114-15^{\circ}$  (18.4 g.), refluxed 3 hrs. with 13.5 g.  $\text{CH}_2(\text{CO}_2\text{H})_2$  in 100 cc. pyridine and 1 cc. piperidine, poured into an excess aqueous  $\text{H}_2\text{SO}_4$ , and the resulting precipitate decarboxylated by heating 1 hr. with 100 cc.  $\text{Ac}_2\text{O}$  gave 52%  $\text{Ph}(\text{CH:CH})_4\text{CO}_2\text{H}$ , yellow leaflets, m.  $213-14^{\circ}$  (from AcOH, then xylene), whose acid chloride (hygroscopic crystals) with the K derivative of IX in xylene gave 68% of the 9- $\text{Ph}(\text{CH:CH})_4\text{CO}$  derivative (XIII) of IX, yellow needles, m.  $190.5-91.5^{\circ}$  (after crystallization from AcOEt, followed by solution in  $\text{HCONMe}_2$  and precipitation with alc.). The K derivative of IX and  $\text{HO}_2\text{CCH}_2\text{COCl}$  gave the 9-carboxyacetyl derivative (XIV) of IX, m.  $135-7^{\circ}$  (loss of  $\text{CO}_2$ ) (from

Et<sub>2</sub>O, precipitated with petr. ether). Ph(CH:CH)<sub>3</sub>CHO and XIV in cold pyridine, treated with a few drops each of piperidine and AcOH and heated 2 hrs. at 70-80°, gave CO<sub>2</sub> and (after cooling to 0°) XIII. Reduction of 10 millimoles XIII in 30 cc. IIIa with 2.5 cc. molar VIII in Et<sub>2</sub>O gave after acidification and CHCl<sub>3</sub> extraction, 1.42 g. IX and, in the extract, 1.7

g.

Ph(CH:CH)<sub>4</sub>CHO (XV), carmine, m. 141-3° (after sublimation at 130° and 0.1 mm.); phenylhydrazone, m. 224-6° (from HCONMe<sub>2</sub>). The reduction of XIII was also carried out with other hydrides, giving the following yields (%) of XV: with I 69, III 68, Li(ZnHPh<sub>2</sub>) 45, and Li(BeHPh<sub>2</sub>), 37. XV was separated from its contaminants by the use of Girard reagent D. In all cases 74-80% IX was also isolated. XIV and Ph(CH:CH)<sub>5</sub>CHO, m. 181-3°, under the above conditions, gave the Ph(CH:CH)<sub>6</sub>CO derivative of IX, dark red needles, m. 206-7° (from HCONMe<sub>2</sub>), which was reduced with VIII to 91% IX and 60% Ph(CH:CH)<sub>6</sub>CHO, carmine, m. 210-13° (subliming at 180° and 0.01 mm.) [phenylhydrazone, m. about 250° (decomposition)]. AcONMe<sub>2</sub> failed to react with PhCH:CHCHO in the presence of EtOK. The 9-Ac derivative of IX treated with PhCH:CHCHO and KOEt at 0° followed by acidification in EtOH, gave 94% IX and only about 1% (impure) XII. On the other hand, PhCH:CHCHO and 9-acetyl-4-nitrocarbazole (XVI) in absolute EtOH with KOEt gave, on acidification, 74% 4-NO<sub>2</sub> derivative of IX, m. 208-10°, 14% XVI, and, from the alc. mother liquors, after evaporation, extraction with

Et<sub>2</sub>O,

extraction of the Et<sub>2</sub>O layer (XVII) with aqueous Na<sub>2</sub>CO<sub>3</sub>, and acidification, 21% Ph(CH:CH)<sub>2</sub>CO<sub>2</sub>H, m. 163-4° (from C<sub>6</sub>H<sub>6</sub>). XVII extracted with aqueous NaHSO<sub>3</sub> yielded 62% PhCH:CHCHO. 30 references.

L14 ANSWER 41 OF 49 CAPLUS COPYRIGHT 2007 ACS on STN

TI Diene syntheses. XXIX. Diene syntheses with unsymmetrical addends; the 1,4-disubstituted diene type

AN 1951:26934 CAPLUS

DN 45:26934

OREF 45:4686d-i,4687a-f

TI Diene syntheses. XXIX. Diene syntheses with unsymmetrical addends; the 1,4-disubstituted diene type

AU Alder, Kurt; Schumacher, Marianne; Wolff, Oswald

CS Univ. Cologne, Germany

SO Ann. (1950), 570, 230-50

DT Journal

LA Unavailable

OS CASREACT 45:26934

AB The 1,4-substituted dienes used in these expts. were all of the trans, trans form. PhCH:CHCH:CHMe (I) (24 g.) and 18 g. CH<sub>2</sub>:CHCO<sub>2</sub>H (II) with traces of o-C<sub>6</sub>H<sub>4</sub>(OH)<sub>2</sub> in 100 cc. PhMe refluxed 6 hrs. gave a mixture of the following 3 isomers (in the ratio of 8:1:1): 2-cis-Phenyl-5-cis-methyl-Δ<sup>3</sup>-tetrahydro-cis-benzoic acid (III), m. 159° (from AcOEt) (the main product); a 3-phenyl-6-methyl-Δ<sup>4</sup>-tetrahydrobenzoic acid (IV), m. 144-6° (from MeCN); and, from the mother liquors of IV, the 2-cis-phenyl-5-cis-methyl-Δ<sup>4</sup>-tetrahydro-trans-benzoic acid (V), m. 90-1° (from AcOEt). Dehydrogenation of III with S at 230-40° gave the new 2,5-PhMeC<sub>6</sub>H<sub>3</sub>CO<sub>2</sub>H, m. 155° (from MeCN), the crude acid chloride of which, refluxed 3.5 hrs. in 100 cc. CS<sub>2</sub> with pure AlCl<sub>3</sub>, gave 2-methyl-9-fluorenone, m. 92° (cf. Kruber, C.A. 26, 5936). Catalytic hydrogenation of III gave a cis-dihydro derivative (VI), C<sub>14</sub>H<sub>18</sub>O<sub>2</sub>, m. 135-6°. The Me ester of VI refluxed with EtONa gave the trans-isomer of VI, m. 87° (also formed by the catalytic hydrogenation of V). Dehydrogenation of IV gave the new 3,6-PhMeC<sub>6</sub>H<sub>3</sub>CO<sub>2</sub>H, m. 209-10°. Catalytic hydrogenation of IV gave the dihydro derivative, C<sub>14</sub>H<sub>18</sub>O<sub>2</sub>, m. 142-3°. MeCH:CHCH:CHCO<sub>2</sub>H (VII) (11.2 g.), 8 g. II, and a trace of o-C<sub>6</sub>H<sub>4</sub>(OH)<sub>2</sub>, heated 5 hrs. at 135°, yielded (after digestion with Me<sub>2</sub>CO) small amts. of insol. polymers and approx. equal-amts. of the mechanically separated 5-cis-methyl-Δ<sup>3</sup>-tetrahydro-

cis,cis-o-phthalic acid (VIII), m. 193-4°, and  
 6-cis-methyl-Δ4-tetrahydro-cis,cis-isophthalic acid (IX), m.  
 174° (both from AcOEt), together with small amts. of an oil, which,  
 when dehydrogenated, gave only 2,4-(HO2C)2C6H3Me. Dehydrogenation of VIII  
 gave 3,4-(HO2C)2C6H3Me. Hydrogenation of VIII gave the saturated cis-dihydro  
 derivative, C9H14O4, m. 173° (decomposition), which when heated 5 hrs. at  
 180° with 20 parts fuming HCl gave the trans-isomer, m.  
 176°, markedly depressing the m.p. of the cis form. The di-Me  
 ester of VIII (properties not given), refluxed with 10% EtONa in EtOH,  
 followed by acidification, gave an isomeric "C-acid" (X), C9H12O4, m.  
 228° (after Et2O extraction and crystallization from AcOEt), giving a new  
 trans-dihydro derivative, m. 178-9°, marked by depressing the m.p. of  
 other dihydro derivs. Dehydrogenation of IX gave 2,4-(HO2C)2C6H3Me (di-Me  
 ester, m. 79°). With NaOEt (as above) IX was in small part  
 converted into the isomeric "m-D-acid" (XI), m. 276-8° (cf.  
 Wagner-Jauregg and Helmert, C.A. 33, 1269.3, who give 280°).  
 Hydrogenation of IX gave a dihydro derivative, m. 195-6°, which with  
 fuming HCl was rearranged into the isomeric dihydro derivative of XI, m.  
 202-3° (also obtained by direct hydrogenation of XI). These  
 rearrangements are discussed, but not fully explained. Refluxing the acid  
 chloride (XII) of VII with CH2:CHCOCl 7 hrs. in PhMe (or in a bomb tube at  
 125°), followed by addition of H2O, yielded a mixture of VIII and IX  
 (but no XI). Similarly, refluxing in xylene, followed by distillation and  
 hydrolysis, gave a mixture of 4 acids: 60% XI (crystallizing directly from the  
 aqueous  
 hydrolyzate) and (on concentrating the aqueous solution), VIII, X, and a small  
 amount of  
 an (unanalyzed) acid, m. 208°, as well as an oil, which  
 dehydrogenated to 2,4-(HO2C)2C6H3Me. XII and CH2:CHCOCl heated at  
 155° in a bomb tube gave results similar to those obtained in  
 xylene (with somewhat improved yields). The Me ester of VII and  
 CH2:CHCO2Me with a trace of o-C6H4(OH)2, heated 5 hrs. at  
 145-50° gave a product (XIII), b13 156-60°, saponified to XI.  
 Hydrogenation of XIII in AcOEt, and saponification gave dihydro derivs. of VIII  
 and IX, in approx. equal amts., and small amts. of an oil, dehydrogenated  
 to 3,4-(HO2C)2C6H3Me. trans,trans-PhCH:CHCH:CHCOCl (10 g.) and 10 g.  
 CH2:CHCOCl kept 30 days at room temperature, then vigorously stirred with Me2CO  
 and H2O, yielded (besides 5 g. PhCH:CHCH:CHCO2H, m. 164°), 4.5 g.  
 4-cis-phenyl-Δ5-tetrahydro-cis,cis-isophthalic acid (XIV), m.  
 222° (from aqueous AcOH). The same reactants (18 g. and 11 g., resp.)  
 heated 72 hrs. at 90-100°, followed by hydrolysis, formed 80% XIV  
 (with no evidence of another isomer). When, however, the reactants were  
 heated in a sealed tube at 120-30°, 60% of the products was an  
 isomer (XV) of XIV, m. 245° (from MeCN). AcCl or Ac2O and XIV  
 yielded the anhydride, C14H12O3, m. 183° (from PhMe), readily  
 reconverted into XIV. Catalytic hydrogenation of XIV gave  
 4-cis-phenylhexahydro-cis,cis-phthalic acid C14H16O4 (XVI), m. 213°  
 (from 50% AcOH); anhydride, m. 156° (from PhMe); di-Me ester, m.  
 50-1° (from MeOH). XVI (2 g.) heated 6 hrs. at 180° with  
 excess fuming HCl gave a mixture of 2 trans isomers, the complete structures  
 of which are still in doubt, but both of which are 4-  
 phenylhexahydroisophthalic acids, 1.5 g. of the isomer (XVII) m.  
 210° and 0.5 g. of the isomer (XVIII) m. 183°.  
 Hydrogenation of XV with PtO2 in AcOH yielded XVIII, which on  
 dehydrogenation with SeO2 in AcOH gave 3,4-(HO2C)2C6H3Ph (XIX), m.  
 245° (from AcOEt and C6H6). Attempts to cause anhydride formation  
 by heating XIX with AcCl gave a noncryst. glassy material reconverted by  
 long heating with H2O into XIX. Dehydrogenation of XV gave XIX. SOCl2 (5  
 cc.) and 0.3 g. AlCl3 refluxed 2 hrs. with 0.5 g. XIX in 20 cc. CS2,  
 followed by rapid stirring with ice-H2O-HCl and by Et2O extraction, formed  
 2-carboxy-9-fluorenone, subliming above 270°, identified as the Me  
 ester, silky needles, m. 181° (from MeOH) [cf. Fortner, Monatsh.  
 25, 451(1904)].

L14 ANSWER 47 OF 49 CAPLUS COPYRIGHT 2007 ACS on STN

TI General synthesis of  $\alpha$ -unsaturated acids from malonic acid

AN 1925:19147 CAPLUS

DN 19:19147

OREF 19:2475d-f

TI General synthesis of  $\alpha$ -unsaturated acids from malonic acid

AU Dutt, I. Sikhibhushan

SO Quart. J. Chem. Soc. (1925), 1, 297-301

DT Journal

LA Unavailable

AB  $\text{CH}_2(\text{CO}_2\text{H})_2$  easily condenses with aldehydes in the presence of  $\text{C}_5\text{H}_{11}\text{N}$  in  $\text{C}_5\text{H}_5\text{N}$  solution to alkylidene- and arylidenemalonic acids, which, under the influence of  $\text{C}_5\text{H}_5\text{N}$ , particularly on heating, lose  $\text{CO}_2$ , giving  $\alpha$ -unsatd.  $\text{CO}_2\text{H}$  acids in excellent yields. AcH gives 75% of crotonic acid; 10 g. glyoxylic acid gives 1.8 g. fumaric and 2.8 g. maleic acids; BzH gives 90% of cinnamic acid; p-MeC<sub>6</sub>H<sub>4</sub>CHO gives 87% p-methylcinnamic acid; furfural gives 70% furfural acrylic acid; o-O<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>CHO gives 73% o-nitrocinnamic acid; the p- and m-derivs. result in 82% and 90%, resp.; piperonal gives 76% piperonylacrylic acid; p-MeOC<sub>6</sub>H<sub>4</sub>CHO gives 80% p-methoxycinnamic acid; p-Me<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>CHO gives 65% p-dimethylaminocinnamic acid; m-BrC<sub>6</sub>H<sub>4</sub>CHO gives 83% of m-bromocinnamic acid; o-HOC<sub>6</sub>H<sub>4</sub>CHO gives 20% o-coumaric acid; carbethoxyvanillin gives 12% of ferulic acid; dicarbethoxyprotocatechualdehyde gives 7% caffeic acid; PhCH:CHCHO (heating the reaction mixture 2 hrs.) gives 70% of cinnamylidenemalonic acid; on longer heating 60% of the cinnamylideneacetic acid. Me<sub>2</sub>CO gives 60% of  $\beta$ , $\beta$ -dimethylacrylic acid; Et<sub>2</sub>CO gives 35% of  $\beta$ , $\beta$ -diethylacrylic acid; cyclohexanone gives not over 5% of cyclohexylideneacetic acid.

L14 ANSWER 48 OF 49 CAPLUS COPYRIGHT 2007 ACS on STN

TI Polymerization of allyl cinnamalacetate

AN 1923:15035 CAPLUS

DN 17:15035

OREF 17:2419e-g

TI Polymerization of allyl cinnamalacetate

AU Blicke, F. F.

SO Journal of the American Chemical Society (1923), 45, 1562-6

CODEN: JACSAT; ISSN: 0002-7863

DT Journal

LA Unavailable

AB Allyl cinnamalacetate (I), obtained in 45-50% yield from allyl alc., PhCH:CHCH:CHCO<sub>2</sub>H (II) and H<sub>2</sub>SO<sub>4</sub> at 90-5°, is light yellow, highly refractive,  $n_D^{20}$  1.5035, is readily saponified by alc. KOH, instantly decolorizes Br in CS<sub>2</sub> and KMnO<sub>4</sub> in H<sub>2</sub>O; hexabromide, m. 126°, seps. from alc. in solvated crystals, m. 111-2°. Heated in small evacuated bulbs for 7 days at 210°, I gradually becomes more and more viscous and finally changes into a light yellow, almost solid mass which, dissolved in Me<sub>2</sub>CO and poured into much cold alc., gives 25% of an amorphous, amber-like polymer of I; this in boiling Me<sub>2</sub>CO with 5 equivs. alc. KOH (calculated on the basis of the monomol. I) gives a slightly yellow amorphous polymer of II; heated with anhydrous Ba(OH)<sub>2</sub> this acid gives a mixture of liquid compds., undoubtedly hydrocarbons, which decolorizes Br and KMnO<sub>4</sub> and therefore contains at least 1 unsatd. constituent. Com. grades of allyl alc. and chloride undergo spontaneous polymerization on long standing.

L14 ANSWER 49 OF 49 CAPLUS COPYRIGHT 2007 ACS on STN

TI The distillation products of  $\alpha$ -truxilic acid. Obtainment of a fourth truxillic acid

AN 1923:15034 CAPLUS

DN 17:15034

OREF 17:2419c-e

TI The distillation products of  $\alpha$ -truxillic acid. Obtainment of a fourth truxillic acid

AU Stobbe, Hans; Zschoch, Fritz

SO Berichte der Deutschen Chemischen Gesellschaft [Abteilung] B: Abhandlungen (1923), 56B, 676-8

CODEN: BDCBAD; ISSN: 0365-9488

DT Journal

LA Unavailable

AB Distillation of four 30-g. portions of  $\alpha$ -truxillic acid gave at 90-190° 1.6 g. of a colorless aqueous liquid, at 190-290° 26.6 g. of (chiefly) trans-cinnamic acid, at 290-320° 50.7 g. of a mixture of stilbene, a compound m. 192-4°,  $\gamma$ -truxillic anhydride (m. 189-90°) and a new  $\eta$ -truxillic anhydride (I), above 320°, with much decomposition, 3.4 g. of a yellow-red liquid containing H<sub>2</sub>O and tarry products, and 18.1 g. residue. I, m. 287°, depresses the m. p. of truxone (m. 294°) 30°, does not give the blue KOH melt typical of truxone, mol. weight in boiling C<sub>6</sub>H<sub>6</sub> 271-8, does not decolorize KMnO<sub>4</sub> in Na<sub>2</sub>CO<sub>3</sub>, at 0°, is only slightly soluble in NaOH, gives with piperidine what is probably  $\eta$ -truxillpiperididic acid, m. 240°, neutral to litmus. Digested a long time with Ba(OH)<sub>2</sub> I gives  $\eta$ -truxillic acid, m. 260° (278-80° if previously heated a long time at 150-60° markedly depresses the m. p. of the  $\alpha$ -acid. Liebermann's "distyryl" (Ber. 22, 124(1889)) is the above mixture of 4 compds. contained in the 290-320° fraction. Distillation of 50 g. trans-cinnamic acid gave: (1) Up to 280°, chief fraction, containing 30 g. cinnamic acid and 3 g. of a neutral portion separated by further fractionation into styrene and stilbene; (2) from 280° to 310°, 1 g. of a resinous mass; (3) 8 g. of carbonized residue.

=> d 114 28-38 ti

L14 ANSWER 28 OF 49 CAPLUS COPYRIGHT 2007 ACS on STN

TI Ethylenes

L14 ANSWER 29 OF 49 CAPLUS COPYRIGHT 2007 ACS on STN

TI Synthesis and properties of  $\alpha,\beta$ -unsaturated valerolactams

L14 ANSWER 30 OF 49 CAPLUS COPYRIGHT 2007 ACS on STN

TI Use of the Wittig reaction for synthesis of  $\alpha,\beta$ -unsaturated and polyene acids

L14 ANSWER 31 OF 49 CAPLUS COPYRIGHT 2007 ACS on STN

TI Synthesis of  $\beta$ -hydroxy esters from ethyl acetate and ketones or aldehydes by means of lithium amide. Some results with other esters

L14 ANSWER 32 OF 49 CAPLUS COPYRIGHT 2007 ACS on STN

TI Several dichlorobutadienyl alcohols and their transformation into dienic acids

L14 ANSWER 33 OF 49 CAPLUS COPYRIGHT 2007 ACS on STN

TI Phosphorus organic compounds. XX. Phosphine oxides as reagents for olefin formation

L14 ANSWER 34 OF 49 CAPLUS COPYRIGHT 2007 ACS on STN

TI Rearrangement of 1,1-dichloro-5-hydroxy(chloro)-5-aryl-1,3-pentadienes into  $\delta$ -arylpentadienoic acids

L14 ANSWER 35 OF 49 CAPLUS COPYRIGHT 2007 ACS on STN

TI The hydrolysis of  $\gamma$ -cyano- $\gamma$ -phenylpimelodinitrile

L14 ANSWER 36 OF 49 CAPLUS COPYRIGHT 2007 ACS on STN

TI The reaction of acetals with malonic acid and its derivatives. A

contribution to the knowledge of the Knoevenagel-Doebner reaction

L14 ANSWER 37 OF 49 CAPLUS COPYRIGHT 2007 ACS on STN  
TI Some new derivatives of khellin and its product of demethylation

L14 ANSWER 38 OF 49 CAPLUS COPYRIGHT 2007 ACS on STN  
TI An attempted synthesis of 1,10-cyclopentenoheptalene. 1,8-Tetramethyleneazulene

=> d l14 30 ti fbib abs

L14 ANSWER 30 OF 49 CAPLUS COPYRIGHT 2007 ACS on STN  
TI Use of the Wittig reaction for synthesis of  $\alpha,\beta$ -unsaturated and polyene acids  
AN 1961:7620 CAPLUS  
DN 55:7620  
OREF 55:1420b-d  
TI Use of the Wittig reaction for synthesis of  $\alpha,\beta$ -unsaturated and polyene acids  
AU Kucherov, V. F.; Kovalev, B. G.; Nazarova, I. I.; Yanovskaya, L. A.  
CS N. D. Zelinskii Inst. Org. Chem., Moscow  
SO Izvestiya Akademii Nauk SSSR, Seriya Khimicheskaya (1960) 1512-14  
CODEN: IASKA6; ISSN: 0002-3353  
DT Journal  
LA Unavailable  
AB cf. W. and Haag, CA 50, 10030g. Refluxing 16.06 g. Ph3P:CHCO2Et with 2.64 g. cinnamaldehyde in C6H6 6 hrs. under N gave after treatment with petr. ether 2.85 g. Et 4-phenyl-1,3-butadienecarboxylate, 70.5%, b1 149-51°, n20D 1.5201; free acid m. 166-7°. Similarly were prepared: 48.5% EtCH:CHCO2Et, b17 54.5-5°, n21D 1.4310; 50% EtOCH2CH2CH:CHCO2Et, b7 73-6°, n19D 1.4427; 100% PhCH:CHCO2Et, b10 138-40°, n20D 1.5591; 50.6% (2-C4H3O)CH:CHCO2Et, b6 100°, n17D 1.5438; 67.5% Me2C:CH(CH2)2CMe:CHCH:CHCO2Et, b14 152-5°, n20D 1.5292; 34.1% CH2:CHCH:CHCO2Et, b19 60-1°, n21D 1.4819 (free acid m. 72°); 80.3% Me(CH:CH)2CO2Et, b8 71-2°, n21D 1.4940; 87% Me(CH:CH)3CO2Et, b0.3 61-3°, m. 39-40° (free acid m. 187-91°); 82% Me(CH:CH)4CO2Et, m. 90-3.5°; 88% Me(CH:CH)5CO2Et, m. 135-6°. Reaction with MeCHBrCHO gave 64.7% MeCHBrCH:CHCO2Et, b4 74-5°, n20D 1.4876. 2,4,6,8-Dodecatetraenecarboxylic acid, m. 226-7°, was prepared by saponification of the Et ester with aqueous MeOH solution of NaOH.

=> logoff hold

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
85.34	228.89

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
-8.58	-14.82

CA SUBSCRIBER PRICE

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PASSWORD:

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FILE 'CAPLUS' ENTERED AT 07:09:44 ON 11 DEC 2007  
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FULL ESTIMATED COST	85.34	228.89
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-8.58	-14.82

=> d his

(FILE 'HOME' ENTERED AT 06:07:53 ON 11 DEC 2007)

L1 FILE 'REGISTRY' ENTERED AT 06:08:12 ON 11 DEC 2007  
0 2,4-PENTADIENEOIC ACID/CN  
E 2,4-PENTADIENEOIC ACID/CN  
E 2,4-PENTADIENEOIC ACID/CN  
E 2,4-PENTADIENEOIC ACID, 5-METHYL/CN  
L2 STRUCTURE UPLOADED  
L3 0 SEARCH L2 EXACT SAM  
L4 3 SEARCH L2 EXACT FULL

L5 FILE 'CAPLUS' ENTERED AT 06:16:55 ON 11 DEC 2007  
9 L4

FILE 'REGISTRY' ENTERED AT 06:27:46 ON 11 DEC 2007

FILE 'CAPLUS' ENTERED AT 06:28:11 ON 11 DEC 2007

L6 FILE 'REGISTRY' ENTERED AT 06:29:04 ON 11 DEC 2007  
E 2,4-PENTADIENEOIC ACID/CN  
1 E3

L7 FILE 'CAPLUS' ENTERED AT 06:29:37 ON 11 DEC 2007  
2 L6/THU

FILE 'REGISTRY' ENTERED AT 06:32:17 ON 11 DEC 2007

L8 FILE 'CAPLUS' ENTERED AT 06:32:27 ON 11 DEC 2007  
33 L6/PREP

L9 FILE 'REGISTRY' ENTERED AT 06:38:10 ON 11 DEC 2007  
E 5-PHENYL- 2,4-PENTADIENEOIC ACID/CN  
E 2,4-PENTADIENEOIC ACID, 5-PHENYL/CN  
2 E4

L10 FILE 'CAPLUS' ENTERED AT 06:39:43 ON 11 DEC 2007  
158 L9  
L11 0 9/THU  
L12 10 L9/THU  
L13 52 L9/PREP  
L14 49 L13 NOT L12

=> d 114 17-27 ti

L14 ANSWER 17 OF 49 CAPLUS COPYRIGHT 2007 ACS on STN

TI Cinnamylideneacetic acid and its derivatives

L14 ANSWER 18 OF 49 CAPLUS COPYRIGHT 2007 ACS on STN  
 TI  $\beta$ -Amyrin juarezate, a novel ester from Marsdenia pringlei and triterpenes from Asclepias linaria

L14 ANSWER 19 OF 49 CAPLUS COPYRIGHT 2007 ACS on STN  
 TI Condensation of ethyl crotonate, 3-methylcrotonate, and isopropylidenemalonate with aromatic aldehydes

L14 ANSWER 20 OF 49 CAPLUS COPYRIGHT 2007 ACS on STN  
 TI Synthesis and NMR and IR spectra of  $\alpha$ -trans- $\gamma$ -cis- $\beta$ -styrylacrylic acid

L14 ANSWER 21 OF 49 CAPLUS COPYRIGHT 2007 ACS on STN  
 TI Condensation of 2-alkyl-substituted salts of 1,3-dioxolanium with aldehyde acetals. Synthesis of unsaturated aromatic and heterocyclic acids

L14 ANSWER 22 OF 49 CAPLUS COPYRIGHT 2007 ACS on STN  
 TI Polyhalogenated  $\alpha,\alpha'$ -diethylenic ketones. Synthesis and properties of polychlorinated 3-pentadienones and 3-heptatrienones

L14 ANSWER 23 OF 49 CAPLUS COPYRIGHT 2007 ACS on STN  
 TI Synthesis of cinnamylideneacetic acid by the Perkin reaction

L14 ANSWER 24 OF 49 CAPLUS COPYRIGHT 2007 ACS on STN  
 TI Use of sulfuric acid as a condensing reagent

L14 ANSWER 25 OF 49 CAPLUS COPYRIGHT 2007 ACS on STN  
 TI Ethyl esters of  $\alpha,\beta$ -unsaturated esters by the PO olefination method

L14 ANSWER 26 OF 49 CAPLUS COPYRIGHT 2007 ACS on STN  
 TI Reactions with phosphinealkylenes. VIII. Novel synthesis of carboxylic acids from phosphine alkylenes

L14 ANSWER 27 OF 49 CAPLUS COPYRIGHT 2007 ACS on STN  
 TI Isomerization of terphenyls

=> d l14 17-20 ti fbib abs

L14 ANSWER 17 OF 49 CAPLUS COPYRIGHT 2007 ACS on STN  
 TI Cinnamylideneacetic acid and its derivatives  
 AN 1975:155832 CAPLUS  
 DN 82:155832  
 OREF 82:24856h,24857a  
 TI Cinnamylideneacetic acid and its derivatives  
 IN Tsuda, Minoru; Tanaka, Hideaki  
 PA Agency of Industrial Sciences and Technology, Japan  
 SO Jpn. Tokkyo Koho, 3 pp.  
 CODEN: JAXXAD  
 DT Patent  
 LA Japanese  
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 49047735	B	19741217	JP 1969-20056	19690318
				JP 1969-20056	19690318
AB	Reaction of 0.5 mole PhCH:CHCHO with 1.5 mole Ac2O over 0.5 mole AcOK at 40° gave 52% PhCH:CHCH:CHCO2H. The large excess of Ac2O inhibited polymerization of the aldehyde and product.				



L14 ANSWER 18 OF 49 CAPLUS COPYRIGHT 2007 ACS on STN  
 TI  $\beta$ -Amyrin juarezate, a novel ester from Marsdenia pringlei and  
 triterpenes from Asclepias linaria  
 AN 1975:54218 CAPLUS  
 DN 82:54218  
 OREF 82:8659a,8662a  
 TI  $\beta$ -Amyrin juarezate, a novel ester from Marsdenia pringlei and  
 triterpenes from Asclepias linaria  
 AU Dominguez, Xorge A.; Marroquin, Jorge; Olguin, Luz M.; Morales, Francisco;  
 Valdez, Victoria  
 CS Dep. Quim., Inst. Tecnol. Estud. Super. Monterrey, Monterrey, Mex.  
 SO Phytochemistry (Elsevier) (1974), 13(11), 2617-18  
 CODEN: PYTCAS; ISSN: 0031-9422  
 DT Journal  
 LA English  
 AB Exts. of M. pringlei, obtained by successive plant treatment with light  
 petrol and EtOH were chromatographed over silica gel, and the  
 chromatograms were eluted with solvents of increasing polarity, starting  
 with C<sub>6</sub>H<sub>6</sub> and proceeding to MeOH, the petrol extract yielding  $\beta$ -amyrin  
 juarezate and the EtOH extract giving kondurite. On hydrogenation,  
 $\beta$ -amyrin 4-phenylvalerate was obtained. The petrol extract of A.  
 linaria was sep. into individual constituents by a combination of column  
 and preparative thin-layer chromatog. yielding triacontane,  
 $\psi$ -taraxasteryl acetate, sitosterol, and oleanolic acid.

L14 ANSWER 19 OF 49 CAPLUS COPYRIGHT 2007 ACS on STN  
 TI Condensation of ethyl crotonate, 3-methylcrotonate, and  
 isopropylidenemalonate with aromatic aldehydes  
 AN 1973:546113 CAPLUS  
 DN 79:146113  
 OREF 79:23681a,23684a  
 TI Condensation of ethyl crotonate, 3-methylcrotonate, and  
 isopropylidenemalonate with aromatic aldehydes  
 AU Angelova, Iordanka; Ivanov, Chavdar  
 CS Chem. Fac., Univ. Kl. Ohridsky, Sofia, Bulg.  
 SO Chemische Berichte (1973), 106(8), 2643-7  
 CODEN: CHBEAM; ISSN: 0009-2940  
 DT Journal  
 LA German  
 GI For diagram(s), see printed CA Issue.  
 AB RC<sub>6</sub>H<sub>4</sub>CHO (R = H, 4-Me, 4-MeO, 2- or 4-Cl) reacted with H<sub>2</sub>NNa and  
 MeCR<sub>1</sub>:CHCO<sub>2</sub>Et (R<sub>1</sub> = H, Me) or Me<sub>2</sub>C:C(CO<sub>2</sub>Et)<sub>2</sub> in DMF to give  
 RC<sub>6</sub>H<sub>4</sub>CH:CHCR<sub>1</sub>:CHCO<sub>2</sub>H or the lactones (I), resp. I were formed via  
 (RC<sub>6</sub>H<sub>4</sub>CH:CH)<sub>2</sub>C:C(CO<sub>2</sub>H)<sub>2</sub>.

L14 ANSWER 20 OF 49 CAPLUS COPYRIGHT 2007 ACS on STN  
 TI Synthesis and NMR and IR spectra of  $\alpha$ -trans- $\gamma$ -cis- $\beta$ -  
 styrylacrylic acid  
 AN 1973:418302 CAPLUS  
 DN 79:18302  
 OREF 79:2939a,2942a  
 TI Synthesis and NMR and IR spectra of  $\alpha$ -trans- $\gamma$ -cis- $\beta$ -  
 styrylacrylic acid  
 AU Stepanova, O. S.; Galatina, A. I.; Nguyen Van Tong  
 CS Odess. Univ., Odessa, USSR  
 SO Voprosy Stereokhimii (1972), No. 2, 109-13  
 CODEN: VSTKB9; ISSN: 0372-6762  
 DT Journal  
 LA Russian  
 AB PhC.tplbond.CCHO reacted with BrCH<sub>2</sub>CO<sub>2</sub>Me in the presence of Zn-C<sub>6</sub>H<sub>6</sub> to  
 give PhC.tplbond.CCH(OH)CH<sub>2</sub>CO<sub>2</sub>Me, which was dehydrated with POC<sub>13</sub> to  
 trans-PhC.tplbond.CCH:CHCO<sub>2</sub>Me (I). Selective hydrogenation of I, followed  
 by hydrolysis, gave  $\alpha$ -trans- $\gamma$ -cis-PhCH:CHCH:CHCO<sub>2</sub>H (II). The

ir and NMR spectra of II were studied.

=> \logoff hold

2 LOGOFF

44626 HOLD

31441 HOLDS

74887 HOLD

(HOLD OR HOLDS)

L15

0 \LOGOFF HOLD

(LOGOFF(W) HOLD)

=> logoff hold

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

106.77

250.32

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

CA SUBSCRIBER PRICE

-11.70

-17.94

SESSION WILL BE HELD FOR 120 MINUTES

STN INTERNATIONAL SESSION SUSPENDED AT 07:12:46 ON 11 DEC 2007

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Welcome to STN International! Enter x:x

LOGINID:SSSPTA1623PAZ

PASSWORD:

\* \* \* \* \* RECONNECTED TO STN INTERNATIONAL \* \* \* \* \*

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FILE 'CAPLUS' ENTERED AT 07:35:03 ON 11 DEC 2007

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COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

106.77

250.32

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

CA SUBSCRIBER PRICE

-11.70

-17.94

=> file reg

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

106.77

250.32

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

CA SUBSCRIBER PRICE

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-17.94

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experimental property data in the original document. For information  
on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=> e 2,4,6-heptatrienoic acid, 5-phenyl/cn

E1	1	2,4,6-HEPTATRIENOIC ACID, 5-METHYL-7-PHENYL-/CN
E2	1	2,4,6-HEPTATRIENOIC ACID, 5-METHYL-7-PHENYL-, ETHYL ESTER/CN
E3	0 -->	2,4,6-HEPTATRIENOIC ACID, 5-PHENYL-/CN
E4	1	2,4,6-HEPTATRIENOIC ACID, 6,7,7-TRICHLORO-, (E,E)-/CN
E5	1	2,4,6-HEPTATRIENOIC ACID, 6,7,7-TRICHLORO-3-HYDROXY-, ETHYL ESTER/CN
E6	1	2,4,6-HEPTATRIENOIC ACID, 6-(((DIMETHYLAMINO)CARBONYL)THIO)- , METHYL ESTER, (2Z,4Z)-/CN
E7	1	2,4,6-HEPTATRIENOIC ACID, 6-(((DIMETHYLAMINO)CARBONYL)THIO)- 7-PHENYL-, METHYL ESTER, (2Z,4E)-/CN
E8	1	2,4,6-HEPTATRIENOIC ACID, 6-(((DIMETHYLAMINO)CARBONYL)THIO)- 7-PHENYL-, METHYL ESTER, (2Z,4Z)-/CN
E9	1	2,4,6-HEPTATRIENOIC ACID, 6-(6-(1,1-DIMETHYLETHYL)-2,3-DIHYD RO-1,1-DIMETHYL-1H-INDEN-4-YL)-, (2E,4E)-/CN
E10	1	2,4,6-HEPTATRIENOIC ACID, 6-(6-(1,1-DIMETHYLETHYL)-2,3-DIHYD RO-1,1-DIMETHYL-1H-INDEN-4-YL)-, METHYL ESTER, (2E,4E)-/CN
E11	1	2,4,6-HEPTATRIENOIC ACID, 6-(6-(1,1-DIMETHYLETHYL)-2,3-DIHYD RO-1,1-DIMETHYL-1H-INDEN-4-YL)-3-METHYL-, (2E,4E)-/CN
E12	1	2,4,6-HEPTATRIENOIC ACID, 6-(6-(1,1-DIMETHYLETHYL)-2,3-DIHYD RO-1,1-DIMETHYL-1H-INDEN-4-YL)-3-METHYL-, METHYL ESTER, (2E, 4E)-/CN

=> e e1

E1	1	2,4,6-HEPTATRIENOIC ACID, 5-METHYL-7-(6,7,7-TRIMETHYL-2,3-DI OXABICYCLO(2.2.2)OCT-5-EN-1-YL)-, METHYL ESTER, (E,E,E)-/CN
E2	1	2,4,6-HEPTATRIENOIC ACID, 5-METHYL-7-(6,7,7-TRIMETHYL-2,3-DI OXABICYCLO(2.2.2)OCT-5-EN-1-YL)-, METHYL ESTER, (E,E,Z)-/CN
E3	1 -->	2,4,6-HEPTATRIENOIC ACID, 5-METHYL-7-PHENYL-/CN
E4	1	2,4,6-HEPTATRIENOIC ACID, 5-METHYL-7-PHENYL-, ETHYL ESTER/CN
E5	1	2,4,6-HEPTATRIENOIC ACID, 6,7,7-TRICHLORO-, (E,E)-/CN
E6	1	2,4,6-HEPTATRIENOIC ACID, 6,7,7-TRICHLORO-3-HYDROXY-, ETHYL ESTER/CN
E7	1	2,4,6-HEPTATRIENOIC ACID, 6-(((DIMETHYLAMINO)CARBONYL)THIO)- , METHYL ESTER, (2Z,4Z)-/CN
E8	1	2,4,6-HEPTATRIENOIC ACID, 6-(((DIMETHYLAMINO)CARBONYL)THIO)- 7-PHENYL-, METHYL ESTER, (2Z,4E)-/CN
E9	1	2,4,6-HEPTATRIENOIC ACID, 6-(((DIMETHYLAMINO)CARBONYL)THIO)- 7-PHENYL-, METHYL ESTER, (2Z,4Z)-/CN
E10	1	2,4,6-HEPTATRIENOIC ACID, 6-(6-(1,1-DIMETHYLETHYL)-2,3-DIHYD RO-1,1-DIMETHYL-1H-INDEN-4-YL)-, (2E,4E)-/CN
E11	1	2,4,6-HEPTATRIENOIC ACID, 6-(6-(1,1-DIMETHYLETHYL)-2,3-DIHYD RO-1,1-DIMETHYL-1H-INDEN-4-YL)-, METHYL ESTER, (2E,4E)-/CN
E12	1	2,4,6-HEPTATRIENOIC ACID, 6-(6-(1,1-DIMETHYLETHYL)-2,3-DIHYD RO-1,1-DIMETHYL-1H-INDEN-4-YL)-3-METHYL-, (2E,4E)-/CN

=> e 2,4,6-heptatrienoic acid, 5-phenyl-/cn

E1	1	2,4,6-HEPTATRIENOIC ACID, 5-METHYL-7-PHENYL-/CN
E2	1	2,4,6-HEPTATRIENOIC ACID, 5-METHYL-7-PHENYL-, ETHYL ESTER/CN
E3	0 -->	2,4,6-HEPTATRIENOIC ACID, 5-PHENYL-/CN
E4	1	2,4,6-HEPTATRIENOIC ACID, 6,7,7-TRICHLORO-, (E,E)-/CN
E5	1	2,4,6-HEPTATRIENOIC ACID, 6,7,7-TRICHLORO-3-HYDROXY-, ETHYL ESTER/CN
E6	1	2,4,6-HEPTATRIENOIC ACID, 6-(((DIMETHYLAMINO) CARBONYL) THIO)-, METHYL ESTER, (2Z,4Z)-/CN
E7	1	2,4,6-HEPTATRIENOIC ACID, 6-(((DIMETHYLAMINO) CARBONYL) THIO)-7-PHENYL-, METHYL ESTER, (2Z,4E)-/CN
E8	1	2,4,6-HEPTATRIENOIC ACID, 6-(((DIMETHYLAMINO) CARBONYL) THIO)-7-PHENYL-, METHYL ESTER, (2Z,4Z)-/CN
E9	1	2,4,6-HEPTATRIENOIC ACID, 6-(6-(1,1-DIMETHYLETHYL)-2,3-DIHYDRO-1,1-DIMETHYL-1H-INDEN-4-YL)-, (2E,4E)-/CN
E10	1	2,4,6-HEPTATRIENOIC ACID, 6-(6-(1,1-DIMETHYLETHYL)-2,3-DIHYDRO-1,1-DIMETHYL-1H-INDEN-4-YL)-, METHYL ESTER, (2E,4E)-/CN
E11	1	2,4,6-HEPTATRIENOIC ACID, 6-(6-(1,1-DIMETHYLETHYL)-2,3-DIHYDRO-1,1-DIMETHYL-1H-INDEN-4-YL)-3-METHYL-, (2E,4E)-/CN
E12	1	2,4,6-HEPTATRIENOIC ACID, 6-(6-(1,1-DIMETHYLETHYL)-2,3-DIHYDRO-1,1-DIMETHYL-1H-INDEN-4-YL)-3-METHYL-, METHYL ESTER, (2E,4E)-/CN

=> e e12

E1	1	2,4,6-HEPTATRIENOIC ACID, 6-(6-(1,1-DIMETHYLETHYL)-2,3-DIHYDRO-1,1-DIMETHYL-1H-INDEN-4-YL)-, METHYL ESTER, (2E,4E)-/CN
E2	1	2,4,6-HEPTATRIENOIC ACID, 6-(6-(1,1-DIMETHYLETHYL)-2,3-DIHYDRO-1,1-DIMETHYL-1H-INDEN-4-YL)-3-METHYL-, (2E,4E)-/CN
E3	1 -->	2,4,6-HEPTATRIENOIC ACID, 6-(6-(1,1-DIMETHYLETHYL)-2,3-DIHYDRO-1,1-DIMETHYL-1H-INDEN-4-YL)-3-METHYL-, METHYL ESTER, (2E,4E)-/CN
E4	1	2,4,6-HEPTATRIENOIC ACID, 6-(ACETYLOXY)-7-PHENYL-, METHYL ESTER, (2Z,4E)-/CN
E5	1	2,4,6-HEPTATRIENOIC ACID, 6-(ACETYLOXY)-7-PHENYL-, METHYL ESTER, (2Z,4Z)-/CN
E6	1	2,4,6-HEPTATRIENOIC ACID, 6-(DIMETHOXYPHOSPHINYL)-, METHYL ESTER, IRON COMPLEX, (E,E)-/CN
E7	1	2,4,6-HEPTATRIENOIC ACID, 6-(HYDROXYMETHYL)-, METHYL ESTER, IRON COMPLEX, (E,E)-/CN
E8	1	2,4,6-HEPTATRIENOIC ACID, 6-FLUORO-3-METHYL-7-(1,2,3,4-TETRAHYDRO-6-QUINOLINYL)-, (2E,4E,6E)-/CN
E9	1	2,4,6-HEPTATRIENOIC ACID, 6-FORMYL-7-((2-(1H-INDOL-3-YL)ETHYL)AMINO)-2-(METHYLTHIO)-, ETHYL ESTER/CN
E10	1	2,4,6-HEPTATRIENOIC ACID, 6-METHYL-, METHYL ESTER/CN
E11	1	2,4,6-HEPTATRIENOIC ACID, 6-METHYL-3-(TRIFLUOROMETHYL)-, ETHYL ESTER, (2E,4E)-/CN
E12	1	2,4,6-HEPTATRIENOIC ACID, 6-METHYL-7-(1H-PYRROL-2-YL)-, ETHYL ESTER/CN

=> e e12

E1	1	2,4,6-HEPTATRIENOIC ACID, 6-METHYL-, METHYL ESTER/CN
E2	1	2,4,6-HEPTATRIENOIC ACID, 6-METHYL-3-(TRIFLUOROMETHYL)-, ETHYL ESTER, (2E,4E)-/CN
E3	1 -->	2,4,6-HEPTATRIENOIC ACID, 6-METHYL-7-(1H-PYRROL-2-YL)-, ETHYL ESTER/CN
E4	1	2,4,6-HEPTATRIENOIC ACID, 6-METHYL-7-(1H-PYRROL-2-YL)-, METHYL ESTER/CN
E5	1	2,4,6-HEPTATRIENOIC ACID, 6-METHYL-7-(1H-PYRROL-2-YL)-, METHYL ESTER, (E,E,E)-/CN
E6	1	2,4,6-HEPTATRIENOIC ACID, 6-METHYL-7-(4-NITROPHENYL)-, ETHYL ESTER, (2E,4E,6E)-/CN
E7	1	2,4,6-HEPTATRIENOIC ACID, 6-METHYL-7-(5-NITRO-2-FURANYL)-, (

		E,E,E)-/CN
E8	1	2,4,6-HEPTATRIENOIC ACID, 6-METHYL-7-(5-NITRO-2-FURANYL)-, M ETHYL ESTER, (E,E,E)-/CN
E9	1	2,4,6-HEPTATRIENOIC ACID, 6-METHYL-7-(TETRAHYDRO-3,4-DIHYDRO XY-2,4,5-TRIMETHYL-2-FURANYL)-, ETHYL ESTER, (2A(2E,4E ,6E),3B,4A,5A)-/CN
E10	1	2,4,6-HEPTATRIENOIC ACID, 6-METHYL-7-(TETRAHYDRO-3,4-DIHYDRO XY-2,4,5-TRIMETHYL-2-FURANYL)-, ETHYL ESTER, (2A(2E,4E ,6E),3B,4A,5A)-(±)-/CN
E11	1	2,4,6-HEPTATRIENOIC ACID, 6-METHYL-7-(TETRAHYDRO-3-HYDROXY-4 -((2-METHOXYETHOXY)METHOXY)-2,4,5-TRIMETHYL-2-FURANYL)-, ETH YL ESTER, (2A(2E,4E,6E),3B,4A,5A)-/CN
E12	1	2,4,6-HEPTATRIENOIC ACID, 6-METHYL-7-(TETRAHYDRO-3-HYDROXY-4 -((2-METHOXYETHOXY)METHOXY)-2,4,5-TRIMETHYL-2-FURANYL)-, ETH YL ESTER, (2A(2E,4E,6E),3B,4A,5A)-(.+ -.)-/CN

=> logoff hold

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION

FULL ESTIMATED COST

2.70	253.02
------	--------

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION

CA SUBSCRIBER PRICE

0.00	-17.94
------	--------

SESSION WILL BE HELD FOR 120 MINUTES

STN INTERNATIONAL SESSION SUSPENDED AT 07:38:44 ON 11 DEC 2007

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSSPAL623PAZ

PASSWORD:

\*\*\*\*\* RECONNECTED TO STN INTERNATIONAL \*\*\*\*\*  
SESSION RESUMED IN FILE 'REGISTRY' AT 07:46:43 ON 11 DEC 2007  
FILE 'REGISTRY' ENTERED AT 07:46:43 ON 11 DEC 2007  
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COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION

FULL ESTIMATED COST

2.70	253.02
------	--------

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

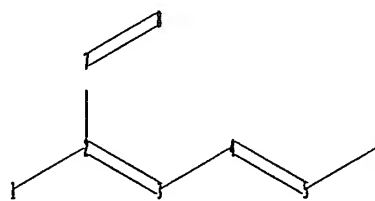
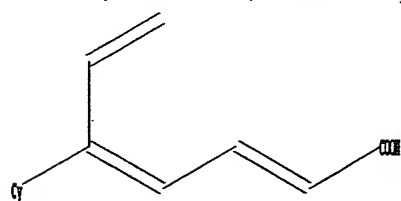
SINCE FILE	TOTAL
ENTRY	SESSION

CA SUBSCRIBER PRICE

0.00	-17.94
------	--------

=>

Uploading C:\Documents and Settings\PZucker\My Documents\Examination Auxillary  
files\10025947\10025947 pt V stab II.str

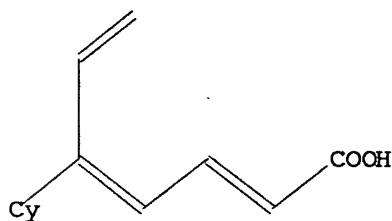


chain nodes :  
1 2 3 4 5 6 7 8  
chain bonds :  
1-2 2-3 2-7 3-4 4-5 5-6 7-8  
exact/norm bonds :  
1-2  
exact bonds :  
2-3 2-7 3-4 4-5 5-6 7-8

Match level :  
1:Atom 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS

L16 STRUCTURE UPLOADED

=> d l16  
L16 HAS NO ANSWERS  
L16 STR



Structure attributes must be viewed using STN Express query preparation.

=> search l16 sss sam  
SAMPLE SEARCH INITIATED 07:47:10 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED - 484 TO ITERATE

100.0% PROCESSED 484 ITERATIONS 0 ANSWERS  
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 8361 TO 10999  
PROJECTED ANSWERS: 0 TO 0

L17 0 SEA SSS SAM L16

=> search l16 sss full  
FULL SEARCH INITIATED 07:47:20 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 9406 TO ITERATE

100.0% PROCESSED 9406 ITERATIONS 3 ANSWERS  
SEARCH TIME: 00.00.01

L18 3 SEA SSS FUL L16

=> d mscan  
'MSCAN' IS NOT A VALID FORMAT FOR FILE 'REGISTRY'

The following are valid formats:

Substance information can be displayed by requesting individual fields or predefined formats. The predefined substance formats are: (RN = CAS Registry Number)

REG - RN  
SAM - Index Name, MF, and structure - no RN  
FIDE - All substance data, except sequence data  
IDE - FIDE, but only 50 names  
SQIDE - IDE, plus sequence data  
SQIDE3 - Same as SQIDE, but 3-letter amino acid codes are used  
SQD - Protein sequence data, includes RN  
SQD3 - Same as SQD, but 3-letter amino acid codes are used  
SQN - Protein sequence name information, includes RN

CALC - Table of calculated properties  
EPROP - Table of experimental properties  
PROP - EPROP and CALC

Any CA File format may be combined with any substance format to obtain CA references citing the substance. The substance formats must be cited first. The CA File predefined formats are:

ABS -- Abstract  
APPS -- Application and Priority Information  
BIB -- CA Accession Number, plus Bibliographic Data  
CAN -- CA Accession Number  
CBIB -- CA Accession Number, plus Bibliographic Data (compressed)  
IND -- Index Data  
IPC -- International Patent Classification  
PATS -- PI, SO  
STD -- BIB, IPC, and NCL

IABS -- ABS, indented, with text labels  
IBIB -- BIB, indented, with text labels  
ISTD -- STD format, indented

OBIB ----- AN, plus Bibliographic Data (original)  
OIBIB ----- OBIB, indented with text labels

SBIB ----- BIB, no citations  
SIBIB ----- IBIB, no citations

The ALL format gives FIDE BIB ABS IND RE, plus sequence data when it is available.

The MAX format is the same as ALL.

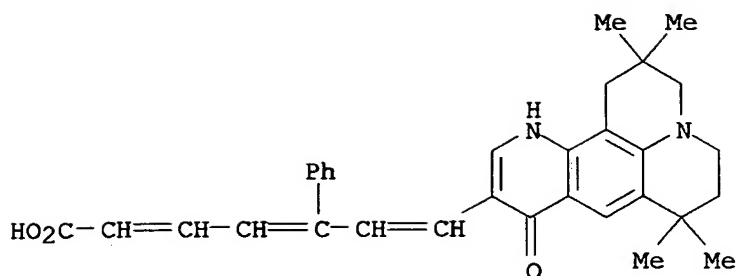
The IALL format is the same as ALL with BIB ABS and IND indented, with text labels.

For additional information, please consult the following help messages:

HELP DFIELDS -- To see a complete list of individual display fields.  
HELP FORMATS -- To see detailed descriptions of the predefined formats.  
ENTER DISPLAY FORMAT (IDE):end

=> d scan

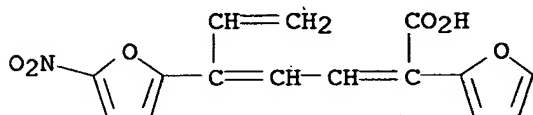
L18 3 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN  
IN 2,4,6-Heptatrienoic acid, 7-(2,3,6,7,9,12-hexahydro-2,2,7,7-tetramethyl-9-oxo-1H,5H-pyrido[3,2,1-gh][1,7]phenanthroline-10-yl)-5-phenyl-  
MF C32 H34 N2 O3



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

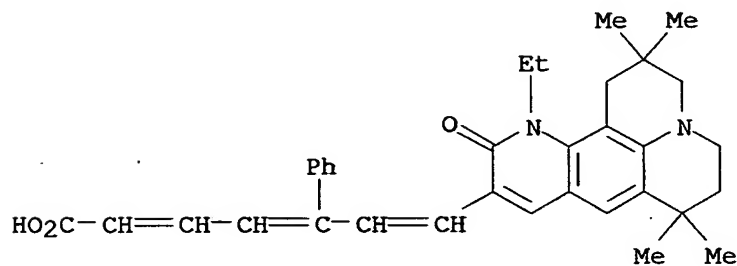
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):3

L18 3 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN  
IN INDEX NAME NOT YET ASSIGNED  
MF C15 H11 N O6



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L18 3 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN  
IN 2,4,6-Heptatrienoic acid, 7-(12-ethyl-2,3,6,7,11,12-hexahydro-2,2,7,7-tetramethyl-11-oxo-1H,5H-pyrido[3,2,1-gh][1,7]phenanthroline-10-yl)-5-phenyl-  
MF C34 H38 N2 O3



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

ALL ANSWERS HAVE BEEN SCANNED

=> logoff hold  
COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION



FULL ESTIMATED COST	176.60	426.92
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-17.94

SESSION WILL BE HELD FOR 120 MINUTES  
STN INTERNATIONAL SESSION SUSPENDED AT 07:49:33 ON 11 DEC 2007

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSSPTA1623PAZ

PASSWORD:

\* \* \* \* \* RECONNECTED TO STN INTERNATIONAL \* \* \* \* \*  
SESSION RESUMED IN FILE 'REGISTRY' AT 08:53:05 ON 11 DEC 2007  
FILE 'REGISTRY' ENTERED AT 08:53:05 ON 11 DEC 2007  
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COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	176.60	426.92
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-17.94

=> e 2,4-pentadienoic acid, 5,5-diphenyl-/cn

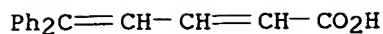
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E2	1	2,4-PENTADIENOIC ACID, 5,5-DIHYDROXY-3-METHYL-2-PROPIONYL-, Δ-LACTONE/CN
E3	1 -->	2,4-PENTADIENOIC ACID, 5,5-DIPHENYL-/CN
E4	1	2,4-PENTADIENOIC ACID, 5,5-DIPHENYL-, (2E)-/CN
E5	1	2,4-PENTADIENOIC ACID, 5,5-DIPHENYL-, (E)-/CN
E6	1	2,4-PENTADIENOIC ACID, 5,5-DIPHENYL-, (Z)-/CN
E7	1	2,4-PENTADIENOIC ACID, 5,5-DIPHENYL-, 4-NITROPHENYL ESTER, (E)-/CN
E8	1	2,4-PENTADIENOIC ACID, 5,5-DIPHENYL-, ETHYL ESTER/CN
E9	1	2,4-PENTADIENOIC ACID, 5,5-DIPHENYL-, ETHYL ESTER, (2E)-/CN
E10	1	2,4-PENTADIENOIC ACID, 5,5-DIPHENYL-, ETHYL ESTER, (2Z)-/CN
E11	1	2,4-PENTADIENOIC ACID, 5,5-DIPHENYL-, ETHYL ESTER, (E)-/CN
E12	1	2,4-PENTADIENOIC ACID, 5,5-DIPHENYL-, ETHYL ESTER, (Z)-/CN

=> e3

L19 1 "2,4-PENTADIENOIC ACID, 5,5-DIPHENYL-/CN

=> d 119

L19 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2007 ACS on STN  
RN 19625-92-4 REGISTRY  
ED Entered STN: 16 Nov 1984  
CN 2,4-Pentadienoic acid, 5,5-diphenyl- (6CI, 8CI, 9CI) (CA INDEX NAME)  
MF C17 H14 O2  
LC STN Files: BEILSTEIN\*, CA, CAOLD, CAPLUS, USPAT2, USPATFULL  
(\*File contains numerically searchable property data)



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

3 REFERENCES IN FILE CA (1907 TO DATE)  
 3 REFERENCES IN FILE CAPLUS (1907 TO DATE)  
 1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	184.40	434.72
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-17.94

FILE 'REGISTRY' ENTERED AT 08:54:20 ON 11 DEC 2007  
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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 10 DEC 2007 HIGHEST RN 957336-90-2  
 DICTIONARY FILE UPDATES: 10 DEC 2007 HIGHEST RN 957336-90-2

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 29, 2007

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

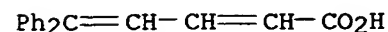
<http://www.cas.org/support/stngen/stndoc/properties.html>

=> 119

L20 1 "2,4-PENTADIENOIC ACID, 5,5-DIPHENYL-"/CN

=> d 120

L20 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2007 ACS on STN  
 RN 19625-92-4 REGISTRY  
 ED Entered STN: 16 Nov 1984  
 CN 2,4-Pentadienoic acid, 5,5-diphenyl- (6CI, 8CI, 9CI) (CA INDEX NAME)  
 MF C17 H14 O2  
 LC STN Files: BEILSTEIN\*, CA, CAOLD, CAPLUS, USPAT2, USPATFULL  
 (\*File contains numerically searchable property data)



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

3 REFERENCES IN FILE CA (1907 TO DATE)  
 3 REFERENCES IN FILE CAPLUS (1907 TO DATE)  
 1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	7.35	442.07

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-17.94

FILE 'CAPLUS' ENTERED AT 08:54:50 ON 11 DEC 2007  
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FILE COVERS 1907 - 11 Dec 2007 VOL 147 ISS 25  
 FILE LAST UPDATED: 10 Dec 2007 (20071210/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

<http://www.cas.org/infopolicy.html>

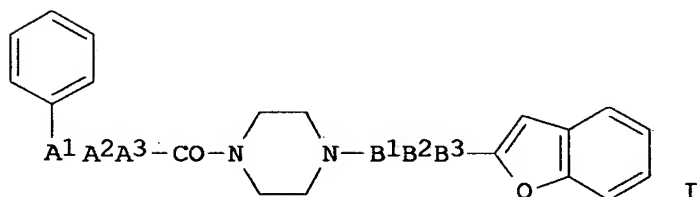
=> l19

L21 3 L19

=> d l21 1-3 ti fbib abs

L21 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN  
 TI Preparation of benzofuran moiety-containing piperazine derivatives as inhibitors of STAT-6 phosphorylation  
 AN 2002:521719 CAPLUS  
 DN 137:93769  
 TI Preparation of benzofuran moiety-containing piperazine derivatives as inhibitors of STAT-6 phosphorylation  
 IN Kawakatsu, Nobuyuki; Namiki, Takayuki; Yamazaki, Norihisa; Yuasa, Masayuki; Miki, Toyohiko; Suenobu, Noriko; Shimanuki, Tomomasa  
 PA Pola Chemical Industries, Inc., Japan  
 SO PCT Int. Appl., 33 pp.  
 CODEN: PIXXD2  
 DT Patent  
 LA Japanese  
 FAN.CNT 1  
 PATENT NO. KIND DATE APPLICATION NO. DATE

PI	WO 2002053550	A1	20020711	WO 2001-JP11265	20011221
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	CA 2439730	A1	20020711	JP 2000-398075	A 20001227
				CA 2001-2439730	20011221
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	AU 2002216388	A1	20020716	WO 2001-JP11265	W 20011221
				AU 2002-216388	20011221
				JP 2000-398075	A 20001227
	EP 1346987	A1	20030924	WO 2001-JP11265	W 20011221
	EP 1346987	B1	20060503	EP 2001-272833	20011221
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
				JP 2000-398075	A 20001227
	AT 325109	T	20060615	WO 2001-JP11265	W 20011221
				AT 2001-272833	20011221
	JP 3990632	B2	20071017	JP 2000-398075	A 20001227
				JP 2002-554669	20011221
				JP 2000-398075	A 20001227
	US 2004053940	A1	20040318	WO 2001-JP11265	W 20011221
	US 6797711	B2	20040928	US 2003-450842	20030626
				JP 2000-398075	A 20001227
				WO 2001-JP11265	W 20011221
OS	MARPAT 137:93769				
GI					



AB The title compds. I [A1 = (CHR1)a; A2 = (CH:CH)q; A3 = (CH2)m; B1 = (CH2)n; B2 = (CR2R3)b; B3 = (CH2)p; R1 is Ph or hydrogen; a is 0 or 1; m, n, b, p, and q are each independently an integer of 0 to 5; and R2 and R3 are each independently hydrogen or hydroxyl, or alternatively R2 and R3 together represent oxygen; a proviso is given] are prepared I inhibit the phosphorylation of STAT 6 and are useful in the treatment or prevention of allergy. The activity of compds. of this invention against JAK-STAT-6 phosphorylation was demonstrated. A formulation is given.

RE.CNT 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L21 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN  
TI 5,5-Diarylpenta-2,4-dienoic acid amides as potential antimalarial agents  
AN 1968:426954 CAPLUS  
DN 69:26954  
OREF 69:5003a,5006a

TI 5,5-Diarylpenta-2,4-dienoic acid amides as potential antimalarial agents  
AU Colwell, William T.; Lange, Judy H.; Henry, David W.  
CS Stanford Res. Inst., Menlo Park, CA, USA  
SO Journal of Medicinal Chemistry (1968), 11, 749-52  
CODEN: JMCMAR; ISSN: 0022-2623

DT Journal

LA English

GI For diagram(s), see printed CA Issue.

AB A series of 5,5-diaryl-penta-2,4-dienoic acids and their amides were synthesized and evaluated as antimalarial agents. The acids were prepared from the corresponding diaryl ketones either directly by a Reformatskii procedure or through acetylenic alc. and acrolein intermediates. The preparation of a series of 3,3-bis(4-chlorophenyl)-acrylamides is also reported. One compound, N,N-diethyl-5,5-bis(4-chlorophenyl)penta-2,4-dienoic acid amide (I), provided significant antiplasmodial activity.

L21 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN

TI Reformatskii reaction in syntheses of  $\omega,\omega$ -diarylalkanoic acids and related compounds

AN 1959:44983 CAPLUS

DN 53:44983

OREF 53:8063b-i,8064a-i

TI Reformatskii reaction in syntheses of  $\omega,\omega$ -diarylalkanoic acids and related compounds

AU Klemm, L. H.; Bower, G. M.

CS Univ. of Oregon, Eugene

SO Journal of Organic Chemistry (1958), 23, 344-8

CODEN: JOCEAH; ISSN: 0022-3263

DT Journal

LA Unavailable

OS CASREACT 53:44983

AB Ph<sub>2</sub>CO and various MeO-substituted benzophenones were submitted to the Reformatskii reaction with BrCH<sub>2</sub>CO<sub>2</sub>Et (I) and BrCH<sub>2</sub>CH:CHCO<sub>2</sub>Me (II), and an attempt made to correlate the data obtained with others quoted in the literature. Following the general procedure of Gardner (C.A. 49, 12358c) 57 g. p-MeOC<sub>6</sub>H<sub>4</sub>CO<sub>2</sub>H and 41 g. MeOPh stirred 2 hrs. at 70° with 540 g. polyphosphoric acid, the mixture poured into ice H<sub>2</sub>O, the precipitate washed with 500 ml. 5% aqueous NaOH and with H<sub>2</sub>O, and the dried product crystallized (alc.) yielded 75-4, g. (p-MeOC<sub>6</sub>H<sub>4</sub>)<sub>2</sub>CO (III), m. 144-6°. Similarly 41 g. 3,4,5-(MeO)<sub>3</sub>C<sub>6</sub>H<sub>2</sub>CO<sub>2</sub>H, 25 g. 1,2-(MeO)<sub>2</sub>C<sub>6</sub>H<sub>4</sub>, and 430 g. polyphosphoric acid gave 36 g. 3,3',4,4',5-pentamethoxybenzophenone (IV). Zn (50 g., 20-mesh activated with HCl), 58.3 g. III, and a crystal of iodine in 400 ml. anhydrous C<sub>6</sub>H<sub>6</sub> stirred under reflux with addition of 70 g. I in 20 ml. C<sub>6</sub>H<sub>6</sub>, the mixture refluxed 15 min. and diluted with 200 ml. 10% AcOH, the aqueous layer extracted with C<sub>6</sub>H<sub>6</sub>, the combined organic solns.

washed (H<sub>2</sub>O,

excess 1.5% NH<sub>4</sub>OH, H<sub>2</sub>O), dried (MgSO<sub>4</sub>), and evaporated gave 55 g.

RR'C(OH)CH<sub>2</sub>CO<sub>2</sub>Et (V, R = R' = p-MeOC<sub>6</sub>H<sub>4</sub>) (VI), m. 92-3° (EtOAc).

VI (14.4 g.) in 140 ml. warm dry C<sub>6</sub>H<sub>6</sub> and 20 ml. anhydrous HCO<sub>2</sub>H refluxed 5

min., the C<sub>6</sub>H<sub>6</sub> removed in a current of air, the residual unsatd. ester

hydrogenated 30 min. in 90 ml. AcOH at 3.5-4.0 atmospheric with 2.5 g. 5% Pd-C,

the filtered solution evaporated, and the residue crystallized yielded 83%

RR'CHCH<sub>2</sub>CO<sub>2</sub>Et (VII, R = R' = p-MeOC<sub>6</sub>H<sub>4</sub>) (VIII), m. 49.5-50.5° (absolute alc.), hydrolyzed 1 hr. by refluxing with 3% KOH in 75% alc., the concentrated solution acidified with HCl, and the precipitate recrystd. (absolute alc.) to

give 97%

RR'CHCH<sub>2</sub>CO<sub>2</sub>H (IX, R = R' = p-MeOC<sub>6</sub>H<sub>4</sub>) (X), m. 138.5-9.5°. Similar

hydrolysis of the residual unsatd. ester (from dehydration of 5 g. VI)

yielded 4.1 g. (p-MeOC<sub>6</sub>H<sub>4</sub>)<sub>2</sub>C:CHCO<sub>2</sub>H, m. 146.5-7.5° (dilute MeOH). IV

and 3-MeOC<sub>6</sub>H<sub>4</sub>Bz were similarly treated in refluxing C<sub>6</sub>H<sub>6</sub> with I. The %

yields for various methoxy-substituted benzophenones in the Reformatskii reaction with I were tabulated for comparison (position of substituents, % yield of V, and over-all % yield of IX given): none, 95, -; 2, 60-70, -;

3, 95-100, 88; 4, 78, 67; 4, 4', 69, 56; 3, 3', 4, 4', 81, -; 3, 4, 4', 5, 70, -; 3, 3', 4, 4', 5, -, 59. From these results it was anticipated that diaryl ketones would react readily with II but with lower yields due to an increasing number of possible side reactions. Zn (4.4 g., activated 20-mesh), 20 g. Ph<sub>2</sub>CO, 55 ml. dry C<sub>6</sub>H<sub>6</sub>, 35 ml. anhydrous Et<sub>2</sub>O, and a crystal of iodine treated in 1 hr. with 10 g. II in 25 ml. C<sub>6</sub>H<sub>6</sub>, the mixture stirred and refluxed 2 hrs. with 2 g. Zn, and treated with 45 ml. 2N AcOH, the organic layer washed (5% aqueous NaHCO<sub>3</sub> and H<sub>2</sub>O), dried (Na<sub>2</sub>SO<sub>4</sub>) and evaporated, the residual oil warmed 15 min. with 2 vols. anhydrous HCO<sub>2</sub>H, the mixture evaporated in a current of air, and the residue fractionally distilled gave 32% Ph<sub>2</sub>C: CHCH:CHCO<sub>2</sub>Me (XI), m. 86-7° (MeOH), refluxed 2 hrs. with a slight excess of 2% KOH in MeOH and the solution acidified to give a quant. yield of Ph<sub>2</sub>C: CHCH: CHCO<sub>2</sub>H, m. 190-1° (PhMe). XI (15 g.) in 150 ml. AcOH hydrogenated 10 min. at 3.5-4.0 atmospheric with 3 g. 5% Pd-C and the filtered solution distilled gave 97% colorless Ph<sub>2</sub>CH(CH<sub>2</sub>)<sub>3</sub>CO<sub>2</sub>Me, b<sub>0.5</sub> 145-50°, hydrolyzed to yield quantitatively Ph<sub>2</sub>CH(CH<sub>2</sub>)<sub>3</sub>CO<sub>2</sub>H, m. 92.5-3.5° (60% alc.), converted by SOCl<sub>2</sub> to the corresponding Ph<sub>2</sub>CH(CH<sub>2</sub>)<sub>3</sub>COCl (XII). XII (from 10 g. acid and 8 ml. SOCl<sub>2</sub>) in 250 ml. purified CS<sub>2</sub> added through the Leonard and Sentz attachment (C.A. 48,676d) in 10 hrs. with stirring and refluxing to 2.7 g. anhydrous AlCl<sub>3</sub> in 750 ml. CS<sub>2</sub> with addns. of 2.7 g. AlCl<sub>3</sub> at 3-hr. intervals, the mixture stirred 2 hrs. and diluted with H<sub>2</sub>O, the organic layer from the filtered mixture distilled and the residue taken up in C<sub>6</sub>H<sub>6</sub>, the washed (excess 10% aqueous K<sub>2</sub>CO<sub>3</sub> and H<sub>2</sub>O), dried (MgSO<sub>4</sub>) solution evaporated, and the residue distilled at 190-200°/0.5 mm. yielded 5.47 g. 9-phenyl-5-benzosuberone (XIII), m. 71.0-1.5° (dilute alc.); oxime, m. 152.5-3.5° (C<sub>6</sub>H<sub>6</sub>-petr. ether). XIII (2 g.) submitted to Huang-Minlon-Wolff-Kishner reduction, the diluted mixture extracted with C<sub>6</sub>H<sub>6</sub>, the H<sub>2</sub>O-washed and dried (MgSO<sub>4</sub>) extract distilled, and the liquid (1.2 g., b<sub>1.0</sub> 132-5°) redistd. gave 5-phenylbenzosuberone (XIV), b<sub>2</sub> 149-50°, m. 41-5°. PhMgBr (0.4 g. Mg, 2.4 g. PhBr, 75 ml. Et<sub>2</sub>O) treated slowly at 0° (ice-bath) with 2 g. 5-benzosuberone (obtained by cyclization of PhCH<sub>2</sub>(CH<sub>2</sub>)<sub>3</sub>CO<sub>2</sub>H with polyphosphoric acid) in 20 ml. Et<sub>2</sub>O, the mixture stirred 30 min. at 0° and refluxed 1 hr., the mixture hydrolyzed and the carbinol dehydrated with HCO<sub>2</sub>H according to Klemm and Ziffer (C.A. 50, 4094f), the product distilled at 1.5 mm. to give 0.4 g. colorless ketonic liquid (presumably starting material) and 1 g. KMnO<sub>4</sub>-reducing liquid. b<sub>1.5</sub> 115-35°, the alkenic fraction (0.9 g.) in 25 ml. AcOH hydrogenated 2 hrs. at 4 atmospheric with 0.1 g. prerduced PtO<sub>2</sub>, and the filtered solution distilled yielded 0.56 g. XIV, b<sub>2</sub> 149-50°, λ 3.26-3.52, 6.24, 6.71, 6.90, 13.35, 13.9, 14.35 μ. XIII (2.36 g.), 1.48 g. HCO<sub>2</sub>Et, and a few ml. C<sub>6</sub>H<sub>6</sub> stirred and warmed with 0.5 g. NaH (N atmospheric), the red paste stirred 1.5 hrs. at 50° in 10 ml. C<sub>6</sub>H<sub>6</sub> and treated successively with 3 ml. AcOH and 30 ml. H<sub>2</sub>O, the H<sub>2</sub>O-washed C<sub>6</sub>H<sub>6</sub> layer extracted with 100 ml. 10% aqueous Na<sub>2</sub>CO<sub>3</sub>, the alkaline extract acidified, and the precipitate recrystd. (EtOAc) gave material, m. 101.5-2.5°, repeatedly recrystd. (C<sub>6</sub>H<sub>6</sub>-ligroine) to give 6-hydroxymethylene-9-phenyl-5-benzosuberone, m. 102.0-2.5°. Attempts to apply the same conditions as used for Reformatskii reaction of II with Ph<sub>2</sub>CO to the reaction of II with the methoxy-substituted benzophenones found to condense readily with I gave only very small quantities of crude resinous products. An alternate pathway to the preparation of diarylvaleric acids was investigated starting with VIII, prepared by the Reformatskii reaction of III with I. LiAlH<sub>4</sub> (3.3 g.) in 400 ml. anhydrous Et<sub>2</sub>O stirred with addition of 29 g. VIII in 110 ml. Et<sub>2</sub>O at a rate to maintain gentle refluxing, the mixture refluxed 1 hr., treated cautiously with EtOAc and 200 ml. cold 3N HCl, the aqueous phase extracted with 150 ml. Et<sub>2</sub>, the combined Et<sub>2</sub>O solns. washed (H<sub>2</sub>O), dried (MgSO<sub>4</sub>) and evaporated, the viscous residue taken up in Et<sub>2</sub>O, and

the solution kept at  $-5^{\circ}$  gave 85% (p-MeOC<sub>6</sub>H<sub>4</sub>)<sub>2</sub>CH(CH<sub>2</sub>)<sub>2</sub>OH (XV), m. 54-5° (Et<sub>2</sub>O); 3,5-dinitrobenzoate, m. 116-17° (C<sub>6</sub>H<sub>6</sub>-ligroine). XV (55 g.) in 250 ml. CCl<sub>4</sub> at  $-5^{\circ}$  stirred with addition in 2 min. of 27 g. freshly distilled PBr<sub>3</sub>, the mixture stirred 30 min. and the solution kept at room temperature overnight, warmed 20 min. at  $50^{\circ}$  and diluted with H<sub>2</sub>O, the aqueous phase extracted with CCl<sub>4</sub>, the combined CCl<sub>4</sub> solns. washed repeatedly with H<sub>2</sub>O, the dried solution (CaCl<sub>2</sub>) evaporated and

the

residue in 200 ml. absolute alc. distilled azeotropically with 20 ml. dry C<sub>6</sub>H<sub>6</sub> until the distilling temperature reached  $78^{\circ}$ , the solution refluxed 5 hrs. with NaCH(CO<sub>2</sub>Et)<sub>2</sub> (from 4.6 g. Na, 350 ml. absolute alc., 32 g. H<sub>2</sub>C(CO<sub>2</sub>Et)<sub>2</sub>), the decanted liquid refluxed 2 hrs. with 28 g. KOH in 100 ml. H<sub>2</sub>O, the mixture concentrated, diluted with H<sub>2</sub>O, washed with Et<sub>2</sub>O and acidified, the

crystalline product

distilled at  $240-70^{\circ}/1$  mm., and the distillate crystallized (EtOAc) gave 31% (p-MeOC<sub>6</sub>H<sub>4</sub>)<sub>2</sub>CH(CH<sub>2</sub>)<sub>2</sub>CO<sub>2</sub>H, m.  $103.5-4.0^{\circ}$ . By the same procedures as used with III, 15 g. Zn, 25 g. IV, and 15 g. I gave V [R = 3,4-(MeO)<sub>2</sub>C<sub>6</sub>H<sub>3</sub>, R' = 3,4,5-(MeO)<sub>3</sub>C<sub>6</sub>H<sub>2</sub>], dehydrated with 50 ml. anhydrous HCO<sub>2</sub>H and the resultant yellow liquid hydrogenated in 200 ml. AcOH with 2 g. 30% Pd-C to give 18 g. VII [R = 3,4-(MeO)<sub>2</sub>C<sub>6</sub>H<sub>3</sub>, R' = 3,4,5-(MeO)<sub>3</sub>C<sub>6</sub>H<sub>2</sub>], m.  $81.5-82.5^{\circ}$  (absolute alc.), hydrolyzed and the product purified by 2 recrystns. (C<sub>6</sub>H<sub>6</sub>-C<sub>6</sub>H<sub>14</sub>) and drying 12 hrs. at  $80^{\circ}/1$  mm. to give the acid IX [R = 3,4-(MeO)<sub>2</sub>C<sub>6</sub>H<sub>3</sub>, R' = 3,4,5-(MeO)<sub>3</sub>C<sub>6</sub>H<sub>2</sub>]. Similarly 15 g. Zn, 21.2 g. p-MeOC<sub>6</sub>H<sub>4</sub>Bz and 25 g. I gave 78% V (R = Ph, R' = p-MeOC<sub>6</sub>H<sub>4</sub>), m.  $79-80^{\circ}$  (EtOAc), converted by dehydration, hydrogenation, and hydrolysis to yield 86% IX (R = Ph, R' = p-MeOC<sub>6</sub>H<sub>4</sub>), m.  $120-2^{\circ}$ . Repetition of the same transformations on 8.5 g. 3-MeOC<sub>6</sub>H<sub>4</sub>Bz produced 9.1 g. crude yellow acid, m.  $92-8^{\circ}$ , recrystd. (EtOAc-petr. ether) to give IX (R = Ph, R' = m-MeOC<sub>6</sub>H<sub>4</sub>), m.  $99-100^{\circ}$ . Following the general procedure of Huang-Minlon (C.A. 41, 1649a), 10 g. BzCH<sub>2</sub>(CH<sub>2</sub>)<sub>2</sub>CO<sub>2</sub>H, 7.5 g. NaOH, 7.5 ml. 95% N<sub>2</sub>H<sub>4</sub>, and 80 ml. (HOCH<sub>2</sub>CH<sub>2</sub>)<sub>2</sub>O gave 8.4 g. PhCH<sub>2</sub>(CH<sub>2</sub>)<sub>2</sub>CO<sub>2</sub>H, m.  $56.6-7.5^{\circ}$  (Et<sub>2</sub>O-petr. ether), identical with the product obtained by Clemmensen reduction of the starting material.

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COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
11.31	453.38

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
-2.34	-20.28

CA SUBSCRIBER PRICE

SESSION WILL BE HELD FOR 120 MINUTES

STN INTERNATIONAL SESSION SUSPENDED AT 08:58:30 ON 11 DEC 2007